

Computational Modeling of Fracture Failure in Mineralized and Prosthetic Biomaterials

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Statement of Originality

This is to certify that to the best of my knowledge, the content of this thesis is my own work. This thesis has not been submitted for any degree or other purposes.

I certify that the intellectual content of this thesis is the product of my own work and that all the assistance received in preparing this thesis and sources have been acknowledged.

Boyang Wan

List of publications

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Abstract

Natural mineralized tissue, such as teeth and bones, consist of hydroxyapatite nanocrystals and traces of water and organic molecules, which have the capacity to tolerate the daily physiological loading, e.g., biting food, body weight. However, due to their high mineralized composition, they have been recognized as a class of relatively brittle biomaterials. The inherent brittle nature and fairly high susceptibility to mechanical failure present a more critical problem in biomedical research field. To replace such diseased or damaged mineralized tissues, prosthetic materials are largely applied in the areas of dental and osteo clinical treatments. Ceramic materials provide numerous favourable characteristics, including biocompatibility and excellent potential to mimic the optical characteristics of natural teeth. In addition to the dental industry, applications of osteofixation/osteosynthesis devices, such as fixation plates, are considered fundamental to stabilize various treatments of bone defects for promoting osteointegration and reconstruction. However, clinical observations and specialized literature have revealed that dental restorative materials and prosthetic fixation devices are often subject to high stress, leading to fracture either by catastrophic overloading or cyclic fatigue failure.

The aim of this thesis is to develop a computational modelling framework on the basis of the extended finite element method (XFEM) to investigate the fracture behaviors of mineralised and synthetic biomaterials in various medical applications. The XFEM modelling results are validated by being compared with the *in-vitro* experiments and/or clinical observations. Through the research in this thesis studies, XFEM has been demonstrated to be a powerful tool to analyse fracture behaviors in the bio-structures not only subjected to static

loadings but also cyclic loadings. The outcomes generated in this thesis help gain some insightful understanding failure of the native or prosthetic structures, which is anticipated to provide some clinical guidelines for the design optimisation of patient-specific prosthetic devices to ensure their reliability and longevity.

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Nomenclature

N_j	Shape function in finite element method
$\mathbf{u}_j$	Nodal displacement vector
$H(x)$	Heaviside function
$\mathbf{a}_j$	Additional degree freedom associated with Heaviside function
$F_\alpha(x)$	Crack tip function
$\mathbf{b}_j$	Additional degree freedom associated with crack tip function
ρ	Density
E	Young's modulus
ν	Poisson's ratio
σ_{uts}	Ultimate tensile stress
σ_Y	Yield strength
Y	Geometrical factor
σ_{MPS}	Maximum principal stress
σ_{vms}	von mises stress
G_I, G_{II}, G_{III}	Strain energy release rate in mode I, II, II respectively
$G_{IC}, G_{IIC}, G_{IIIC}$	Critical strain energy release rate in mode I, II, II respectively
K	Stress intensity factor
$K_{IC}, K_{IIC}, K_{IIIC}$	Fracture toughness in mode I, II, II respectively
A	Material constant in hysteresis energy criterion
B	Material exponent coefficient in hysteresis energy criterion
C	Material constant in Paris law

m	Material exponent in Paris law
U	Strain energy density
$\mathcal{E}$	Mechanical stimulus in bone remodelling
Θ	Reference stimulus value for bone remodelling
C_{ap}	Rate constant for bone apposition
C_{or}	Rate constant for overloading bone resorption
C_{ur}	Rate constant for underloading bone resorption
α	Correlation coefficient
β	Correlation exponent coefficient

Abbreviations

2D	Two dimension/two dimensional
3D	Three dimension/three dimensional
FE	Finite element
FEA	Finite element analysis
XFEM	Extended finite element method
DEM	Discrete element method
CZM	Cohesive zone method
DOF	Degree of freedom
LSM	Level set method
LEFM	Linear Elastic Fracture Mechanics
ASTM	American society for testing and materials
LCF	Low cycle fatigue
HCF	High cycle fatigue
FCG	Fatigue crack growth
SIF	Stress intensity factor
SED	Strain energy density
MPS	Maximum principal stress
CAD	Computer aided design
CAM	Computer aided manufacturing
DIC	Digital image correlation
SEM	Scanning electron microscopy

TEM	Transmission electron microscopy
CT	Computed tomography
MRI	Magnetic resonance imaging
XMT	X-Ray micro tomography
HU	Hounsfield unit
PDL	Periodontal ligament
DEJ	Dentine enamel junction
LP	Lateral pterygoid
T	Temporalis
MP	Medial pterygoid
MA	Masseter
FPD	Fixed partial denture
FFF	Fibular free flap
Y-TZP	Yttrium-stabilized tetragonal zirconia
PICN	polymer infiltrated ceramic network
LDS	Lithium disilicate
FC	Feldspar ceramic
HPP	High performance polymer
HA	Hydroxyapatite
TCP	Tricalcium phosphate
FDM	Functional graded material

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Chapter 1: Introduction

1.1 Overview/background

Mineralised tissues, including teeth and bones, play a key role in sustaining the physiological loads owing to their high hardness and stiffness. Compared to bony tissues, teeth are unique biological structures naturally designed to last for a lifetime, therefore, humans grow no new teeth after the complete eruption of their permanent dentition. Dental enamel, as the most mineralised tissue in the human body, mainly consists of hydroxyapatite nanocrystals and traces of water and organic molecules. The crystalline structure as well as the high hardness and stiffness of enamel impart it with the capacity to tolerate a range of lifelong mechanical, thermal and chemical stimuli while still maintaining its cutting and masticatory functions. However, due to its highly mineralised composition, tooth enamel is a relatively brittle biomaterial with a toughness value comparable to that of glass. The inherent brittle nature and high susceptibility to mechanical failure present a more critical problem in the posterior tooth.

To replace the diseased or injured mineralised tissues, prosthetic materials are primarily focused in the areas of dental and osteo clinical applications. Dental restorative materials have been extensively employed in prosthetic dentistry. Ceramic materials present numerous favorable characteristics, including biocompatibility and excellent potential to simulate the optical characteristics of natural teeth. However, the evaluation of clinical survival rates of posterior restorations reveals the vulnerability of those systems to various failure modes. Therefore, many trials have been attempted to evaluate and improve the fracture strength of

all-ceramic restations, including optimising geometrical design, tooth preparation, material selection, etc.

In addition to the dental industry, applications of osteofixation/osteosynthesis devices, such as fixation plates, are considered fundamental to stabilize various treatments of bone defects for promoting osteointegration and reconstruction. However, clinical observations and specialized literature have revealed that metallic fixation devices are often subject to high stress, potentially leading to fracture either by catastrophic overloading or cyclic fatigue failure.

To investigate the fracture characteristics, physical tests are commonly carried out in practice. Nevertheless, such experimental methods are often too expensive and/or time-consuming, and sometimes difficult to capture important mechanics details. Therefore, more efficient alternatives such as computational modelling approaches are drawing growing attention in the fracture analysis of biomedical structures. The development of more advanced modelling techniques makes it possible to simulate the fracture process efficiently and accurately in prosthetic materials of bio-structures. Through the research in this thesis studies, different forms of extended finite element method (XFEM) have been demonstrated to be a powerful tool for analysing fracture behaviours in various bio-structures. The outcomes generated in this thesis could provide some useful clinical guidelines for design optimisation of patient-specific prosthetic devices to ensure their reliability and longevity.

1.2 Major objectives of thesis

The major goal of this thesis is to develop a computational framework on the basis of the XFEM to investigate the fracture behaviours of mineralised and synthetic biomaterials in

various medical applications. This research is aimed to address the following research questions:

(1) Develop an effective computational method to predict the crack initiation and propagation in various biomedical applications under both static and cyclic loadings.

(2) Study the fracture behaviour of the natural mineralised materials and investigate the relevant anatomical factors on the fracture resistance of the mineralised tissues.

(3) Investigate the correlative effect of the restorative designs and materials on the fracture behaviours.

(4) Develop an efficient numerical framework based on XFEM to predict the fatigue failure of the prosthetic plates under the cyclic physiological loading.

(5) Develop a time-dependent computational approach for more realistically predicting fatigue life of prosthetic devices subject to a tissue remodelling condition *in-silico*.

1.3 Thesis outline

This thesis consists of eight chapters, excluding the chapters of introduction and conclusion, there are six main chapters based on the published journal articles or manuscripts intended for submission. They are summarised as follows.

1.3.1 Chapter 2: Literature review on fracture modelling of brittle materials in biomedical applications

This chapter provides a comprehensive review on the state-of-the-art for computational fracture prediction and modelling of bio-ceramics used in biomedical applications. In this

review, the effects of material properties, geometries and topological configurations on fracture strength of the load-bearing prostheses were discussed in detail. Furthermore, the review provides some insights into the crucial region where fractures could likely occur in the ceramic bio-structures so that the optimum design and material selection could be made more properly.

This chapter is based upon the following manuscript prepared for submission:

Boyang Wan, Chi Wu, Ziyang Man, Qing Li. Fracture modelling of ceramic material in biomedical applications: the state of the art and perspective.

1.3.2 Chapter 3: Modelling of stress distribution and fracture in dental occlusal fissures

This Chapter investigates the fracture behaviours of the dental enamel under simulated occlusal loads in relation to various interacting factors, such as fissure morphology, cuspal angle and the underlying material properties of enamel. The outcomes of this Chapter explain how the interplay of compositional and structural features of enamel in the fissural area contribute to the resistance of the human tooth against masticatory forces.

This Chapter is based upon the following published journal article:

Boyang Wan, Mahdi Shahmoradi, Zhongpu Zhang, Yo Shibata, Babak Sarrafpour, Michael Swain, Qing Li. (2019). Modelling of stress distribution and fracture in dental occlusal fissures. *Scientific reports*, 9(1), 1-10.

1.3.3 Chapter 4: Mechanical failure of posterior due to caries and occlusal wear

This Chapter explores the effect of occlusal wear and different types and degrees of caries on the mechanical performance and structural integrity of posterior teeth. The findings

of this Chapter emphasise the importance of early interventions in the management of caries for the prevention of possible tooth fracture, especially in the subjects with higher risk factors, such as caries, wear and bruxism.

This chapter is based upon the following published journal article:

Mahdi Shahmoradi, **Boyang Wan**, Zhongpu Zhang, Michael Swain, & Qing Li. (2022). Mechanical failure of posterior teeth due to caries and occlusal wear - A modelling study. *Journal of Mechanical Behaviors of Biomedical Materials*, 125, 10492. (Mahdi Shahmoradi and Boyang Wan have equal contribution)

1.3.4 Chapter 5: Effect of restorative materials and structures on monolithic dental crown fracture

This Chapter presents a comprehensive study on the fracture behaviours of ceramic dental monolithic crowns. The numerical results show good agreement with the *in-vitro* experiment tests and fractographical analysis results, and they illustrate the joint effects of the design parameters and materials properties on crown reliability. A mathematical expression is derived based on the simulation results to formulate the relation between failure load and design variables analytically.

This Chapter is based upon the following published journal article:

Mahdi Shahmoradi, **Boyang Wan**, Zhongpu Zhang, Tom Wilson., Michael Swain, & Qing Li. (2020). Monolithic crowns fracture analysis: The effect of material properties, cusp angle and crown thickness. *Dental Materials*. 36(8), 1038-1051. (Mahdi Shahmoradi and Boyang Wan have equal contribution)

1.3.5 Chapter 6: On fatigue failure prediction of prosthetic devices through XFEM analysis

In this Chapter, an XFEM-based computational approach is proposed to study the fatigue crack propagation and lifespan of the fixation plates. The numerical analysis is validated by comparing with the experimental and/or clinical results. The results divulge the importance of the tissue ingrowth and bone healing to the fatigue life of fixation plates. The findings from this work would be used as a clinical guideline and beneficial to design optimization of reconstruction devices to ensure durability.

This Chapter is based upon the following published journal article:

Boyang Wan, Ali Entezari, Zhongpu Zhang, Tom Wilson, Nobuhiro Yoda, Keke Zheng, Chi Wu, Guangyong Sun, Keiichi Sasaki, Michael Swain, Qing Li. (2021). On fatigue failure prediction of prosthetic devices through XFEM analysis. *International Journal of Fatigue*, 106160.

1.3.6 Chapter 7: On interaction between fatigue of reconstruction plate and time-dependent bone remodelling

This Chapter presents a coupled analysis approach for the interaction between bone's ongoing remodelling and fatigue damage of prosthetic reconstruction plate by using a novel XFEM based procedure. The results exhibited the importance of bone remodelling to the fatigue life of fixation plates, and vice versa in a quantitative way. Appropriate remodelling of grafted bony tissues can extend the fatigue life of fixation plates. In turn, fatigue strength of the prosthetic device could help stabilise bone healing and enhance bone remodelling outcomes.

This Chapter is based upon the following published journal article:

Boyang Wan, Nobuhiro Yoda, Keke Zheng, Zhongpu Zhang, Chi Wu, Jonathan Clark, Keiichi Sasaki, Michael Swain, Qing Li. (2022). On interaction between fatigue of reconstruction plate and

time-dependent bone remodeling. *Journal of Mechanical Behaviors of Biomedical Materials*,126, 105483.

Chapter 2: Literature review on fracture modelling of ceramic materials in biomedical applications

The load-bearing prostheses used in hard-tissue engineering are extensively used in the areas of dental and orthopedic clinical applications, which are primarily used for replacing injured, diseased, or abnormal body parts such as teeth, joints, bones etc. From a mechanical standpoint, the prosthetic materials should possess high wear and corrosion resistance, high fracture toughness and fatigue strength. Moreover, they must be made of highly biocompatible alloying elements, as the lack of any or many of these factors may lead to incompatibility between the bony tissue and implant materials. Due to the unsurpassed wear resistance and chemical stability, ceramics are one of the key families of biomaterials widely used in biomedical industry. However, the limitation of ceramic bio-structures in load-bearing applications is related to their inherent behaviour of brittleness, which can lead to catastrophic failure *in vivo*. In this regard, *in-silico* modelling signified an effective and accurate approach to prediction and examination of the fracture behaviours in rather complex bio-structures. Based on the available literature, this Chapter provides a comprehensive review on the computational fracture prediction and modelling of bio-ceramics used in the biomedical applications. In this review, the effects of material properties, geometries and topological configurations on fracture strength of the load-bearing prostheses were discussed in detail. The study aims to provide some insights into the crucial region where fractures are likely to occur in the ceramic bio-structures so that the optimum design and material selection could be made.

2.1 Introduction

Load-bearing hard-tissue engineered prostheses are extensively applied for dental and ortho clinical applications, primarily for replacing injured, diseased, or abnormal body parts such as teeth, joints, bones, etc [1-3]. From a mechanical viewpoint, materials used for the fabrication of a load-bearing implant should possess excellent wear and corrosion resistance, high fracture toughness and fatigue strength. Moreover, they must be fabricated of highly biocompatible alloying elements to ensure compatibility between the bony tissues and implant materials [4]. In other words, these biomaterials should satisfy all the clinical, mechanical, manufacturing, and economic requirements in order to be used for load-bearing applications.

Due to the unsurpassed wear resistance and chemical stability, ceramics are one of the key families of biomaterials usually used in biomedical industry [3, 5, 6], as shown in Figure 2.1. Although metals are characterized by a combination of high strength and moderate plastic deformation that favors their application for bio-structures, ceramics are more bio-inert, which could potentially eliminate metal ion release, thereby avoiding inflammation [7]. In addition, dental applications add aesthetic requirements (color and translucency) to the mechanical and biocompatibility specifications [3]. White to ivory color gives a clear advantage for ceramics versus metals, which is the reason why research and development are nowadays directed towards metal-free prosthetic restorations. However, the limitation of ceramic bio-structures in load-bearing applications is related to their characteristic brittleness, which can lead to catastrophic failure in vivo [3, 8]. The low fracture toughness of ceramics, coupled with their susceptibility to failure by slow crack growth under stresses below their fracture strength, remains a major concern for the reliability of ceramic components.

Therefore, critical quality control to avoid overloading and/or fatigue fracture for medical device applications is essential.



Figure 2.1: Ceramic load-bearing materials used in various biomedical applications [9, 10].

Finite element analysis (FEA) provides an effective computational approach for modelling of engineering problems [11-13]. This approach is crucial for biomedical applications because of the complexity of the shapes and loading of such components. FEA has helped many researchers to identify the crucial regions where high mechanical stresses and strains develop and where fatigue or fracture may lead to prosthesis failure [14, 15]. In addition, FEA can be used to estimate the number of cycles that a prosthesis could survive before the actual failure or yielding [16, 17]. Another advantage of using FEA is its capabilities of optimizing the structural geometry, shape/topology, and material selection to

achieve adequate mechanical strength. On the other hand, tests to confirm such analyses are not easy to conduct experimentally due to complex loading and contact conditions in vivo.

Until recently, linear elastic FEA models have been primarily employed for dental and orthopaedic applications. However, some limitations with linear models, is that genuine relationships between crack growth and applied load cannot be formulated [18]. To overcome this limitation, the conventional FE model has been adapted to enable the simulation of crack initiation and propagation inside a structure as per a Linear Elastic Fracture Mechanics (LEFM) framework. A so called re-meshing technique, about the crack tip, was one of the computational methods first developed to mimic crack propagation in structures [18]. However, re-meshing is computationally expensive in particular for 3D structures because of continuously having to reassign the elemental boundary [18]. Subsequently, more advanced computational techniques have been developed, e.g., XFEM, Phase field, etc., to predict crack initiation and extension in brittle and quasi-brittle materials used in biomedical applications [19, 20].

This study aims to comprehensively review recent advancements in computational modelling for fracture prediction and analysis of ceramic bio-structures, with a focus on ensuring their structural stability and avoiding catastrophic failure. The investigation will also emphasize the contributing factors that influence fracture strength and mechanical behaviours, including material selections, design parameters, and loading conditions, among others. Section 2 presents an overview of various commercial simulation codes and more advanced computational methods, alongside a comparison of common fracture damage criteria based on the available literature. Sections 2.3, 2.4, and 2.5 delve into a thorough examination of published numerical studies on fracture characteristics and predictions of various ceramic

structures in dental, orthopaedic, and bone tissue engineering applications, respectively. Finally, the paper concludes with a state-of-the-art outlook, providing valuable insights to researchers on ensuring structural stability and longevity of ceramic-based load-bearing prostheses in Section 2.6.

2.2 Modelling approaches

2.2.1 Numerical techniques

2.2.1.1 Methodology for the computational simulations in biomechanical system

The development of numerical models needs to capture the geometrical complexity of biomechanical systems. Along with rapid advances in computational science, simulation accuracy and efficiency have greatly improved in commercial simulation programs in recent decades. A typical framework of simulating the fracture behaviour of biostructures is illustrated in Figure 2.2. Firstly, accurate and detailed data of the biomechanical system is acquired through advanced imaging techniques such as computed tomography (CT), magnetic resonance imaging (MRI), 3D surface scanning, etc. The acquired images are then processed using image segmentation to extract the region of interest and construct a 3D geometric model of the system. The model is discretised into finite elements to create a computational mesh, and appropriate material properties are assigned to different components based on their mechanical behavior and biological characteristics. Subsequently, realistic boundary conditions and loading scenarios are applied to simulate the actual biomechanical environment. Numerical analysis, such as finite element analysis (FEA), is employed to solve the equations governing the mechanical behaviour of the system under specific loading conditions. The simulation results are then carefully analyzed to understand mechanical responses of the biomechanical system. Regarding fracture modeling and analysis, the

numerical analysis focuses on calculating stress distributions and strain patterns, which are closely related to the locations that are susceptible to fracture initiation. Selecting the appropriate fracture criteria and failure models are crucial in numerical simulations to ensure accurate prediction of fracture initiation and propagation. The computational model is iteratively refined based on experimental/clinical validation results and sensitivity analysis to enhance accuracy and predictive capabilities. Ultimately, the methodology offers valuable insights into the mechanical behavior and fracture prediction of biomechanical systems, contributing to improved understanding, design optimization, and informed clinical decision-making.

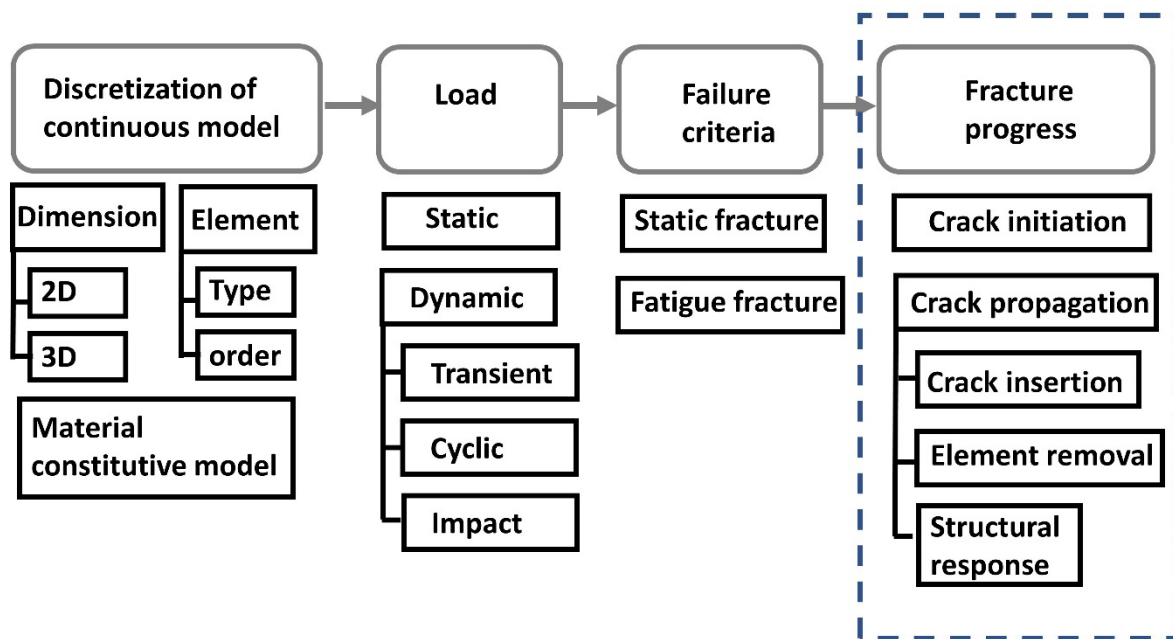


Figure 2.2: Main framework of simulation of fracture behaviors of bio-structures.

2.2.1.2 Common commercial finite element analysis codes

With rapid development in numerical techniques and computer power, computational simulation has been extensively used to examine the mechanical strength of ceramic structures in biomedical engineering. A large number of researchers have commonly utilised FEA to examine the stress distribution in the ceramic structures. Understanding the stress magnitudes and distribution under functional loading helps predict both the possible locations of initial cracking and the overall possibility of failure. The accuracy of simulation results can be affected by various factors, such as analysis types, FE solvers, element types, etc, as summarised in Table 2.1. From the literature, there are four commercial FEA codes that have been commonly used in the field of longevity of bio-ceramic structures, namely ANSYS, ABAQUS, COMSOL, and MSC MARC/NASTRAN.

(a) ANSYS

The flexibility and robust design of ANSYS (ANSYS Incorporation, Canonsburg, PA, USA) make it a versatile FEA code across different disciplines. The multi-physics feature of ANSYS allows the same model to be used for a variety of coupled field applications, e.g., thermal-structural, fluid-structural, etc. For instance, Dawood et al. [1] evaluated the thermal and mechanical induced stresses in the dental restorations via ANSYS. Marques et al. [2] compared the mechanical strength of ceramic scaffolds by considering the nutrition transport. In addition, two useful optimization types, namely parametric design and topology optimization, are implemented in ANSYS. In this regard, Tribst et al. [3] used ANSYS to investigate the main design parameters of dental crowns. Moreover, comprehensive graphical tools are incorporated in ANSYS, allowing for an effective visualisation of simulation results.

(b) ABAQUS

ABAQUS (ABAQUS Incorporation, Johnston, RI, USA) is a commercial FE program, which provides static and dynamic analysis, heat and mass transfer, etc. ABAQUS has been used extensively for many complex engineering problems due to its numerous features such as: a comprehensive library of elements that can be used to model different geometry, compatibility with other computer-aided design (CAD) packages, capacity to perform highly nonlinear and dynamic analyses, etc. Explicit/ABAQUS enables the step increment and convergence tolerance to be calculated automatically to ensure an efficient solution for various non-linear analyses. Furthermore, with the help of user-subroutines, e.g. UMAT/VUMAT, ABAQUS provides great flexibility to model the complex constitutive models of biomaterials on the basis of experimental data.

(c) COMSOL

COMSOL Multiphysics (COMSOL Incorporation, Burlington, MA, USA), known as FEMLAB before 2005, is an FEA solution for complex structural and thermal problems. COMSOL is commonly used to perform coupled engineering analysis involving multiphysics, mechanical, thermal, diffusion etc. A number of studies adopted COMSOL to mimic the thermal-induced stresses in the dental restorations [4-6]. Compared to ANSYS and ABAQUS, COMSOL has a unique element technique, which, to a certain extent reduces the modelling effort, solution time and computer requirements [7].

(d) MSC MARC/NASTRAN

MSC MAR and MSC NASTRAN (MSC Software Corporation, Santa Ana, CA, USA) are general-purpose FEA solutions for various engineering problems. They have some robust nonlinear FEA solvers capable of accurately simulating the behaviour of various products

including complex contact conditions, large deformation and multi-physics interactions. MENTAT and PATRAN are able to enhance the delivery of efficient and complete analysis results (pre-processing and post-processing solution) for an implicit nonlinear FEA. MSC MARC/NASTRAN includes a variety of elements for solving complex problems appropriately. It allows handling product testing and manufacturing simulation, including prediction of damage and crack initiation/propagation.

Table 2.1: Summary on computational modeling codes for structural longevity analysis in biomedical applications.

Analysis type	Software	Element types	Ref.
Static	ABAQUS/standard	4-node bilinear axisymmetric quadrilateral element	[8, 9]
		4-node tetrahedral element	[10-17]
		10-node quadratic tetrahedral element	[18-26]
		8-node linear hexahedral element	[27-30]
		20-node hexahedral elements	[31]
	ANSYS	4 node quadrilateral element	[32]
		4-node tetrahedral element	[33-36]
		10-node quadratic tetrahedral elements	[37-45]
		8-node hexahedral elements	[46-48]
		20-node second-order hexahedral elements	[49]
	FEAST SMT	hexahedron brick elements	[50]
	StressCheck	4-node tetrahedral element	[51]
	FEMAP/CAEFEM	Tetrahedron element	[52, 53]
	Algor Fempro	Tetrahedron element	[54]
		8-node linear hexahedral element	[54-56]
	FACILE	3-node triangular element	[57]
	NX Nastran	10-node tetrahedral element	[58-61]
	MSC Marc	10-node tetrahedron element	[62, 63]
	ADINA	4-node tetrahedron element	[64]

	ALTAIR	4-node tetrahedron element	[65-67]
	SolidWorks	10-node tetrahedron element	[68]
		Hexahedral element	[69]
	COMSOL	Tetrahedron element	[70-73]
Dynamic	ABAQUS/Explicit	4-node liner tetrahedral element	[74-77]
		8-node linear hexahedral element	[28, 29, 78]
	ANSYS	4-node tetrahedral element	[33, 79, 80]
		10-node tetrahedral solid elements	[81]
		8-node linear hexahedral element	[82, 83]
		Second-order hexahedral elements	[49]
	MSC Marc	4-node quadrilateral element	[84]
Transient	ABAQUS/Explicit	4-node tetrahedron element	[14, 85-88]
	ANSYS	10-node tetrahedral element	[1, 89]
		20-node hexahedral elements	[89]
	COMSOL	3-node triangular element	[4]
		Tetrahedral element	[4-6, 90]
	MSC Marc	Hexahedral element	[91]
-	ProMechanica	Tetrahedron element	[85, 92-94]
	Simufact Engineering	4-node tetrahedron element	[95, 96]
	NX Nastran	tetrahedron element	[97-99]
	Rhinoceros	tetrahedral element	[100]

2.2.1.3 Advanced modelling techniques

The development in more advanced modelling techniques enables to simulate the fracture process in ceramic bio-structures. Immense effort has been made over the last two decades to develop accurate and efficient numerical algorithms to model the cracking processes in complex structures in biomedical applications, including eXtended Finite

Element Method (XFEM), Phase-field, Cohesive zone model, Discrete Element Method (DEM), as summarised in Table 2.2. For comparison, a benchmark engineering problem with a 3-Point bending test is simulated by various modelling techniques as shown in Figure 2.3

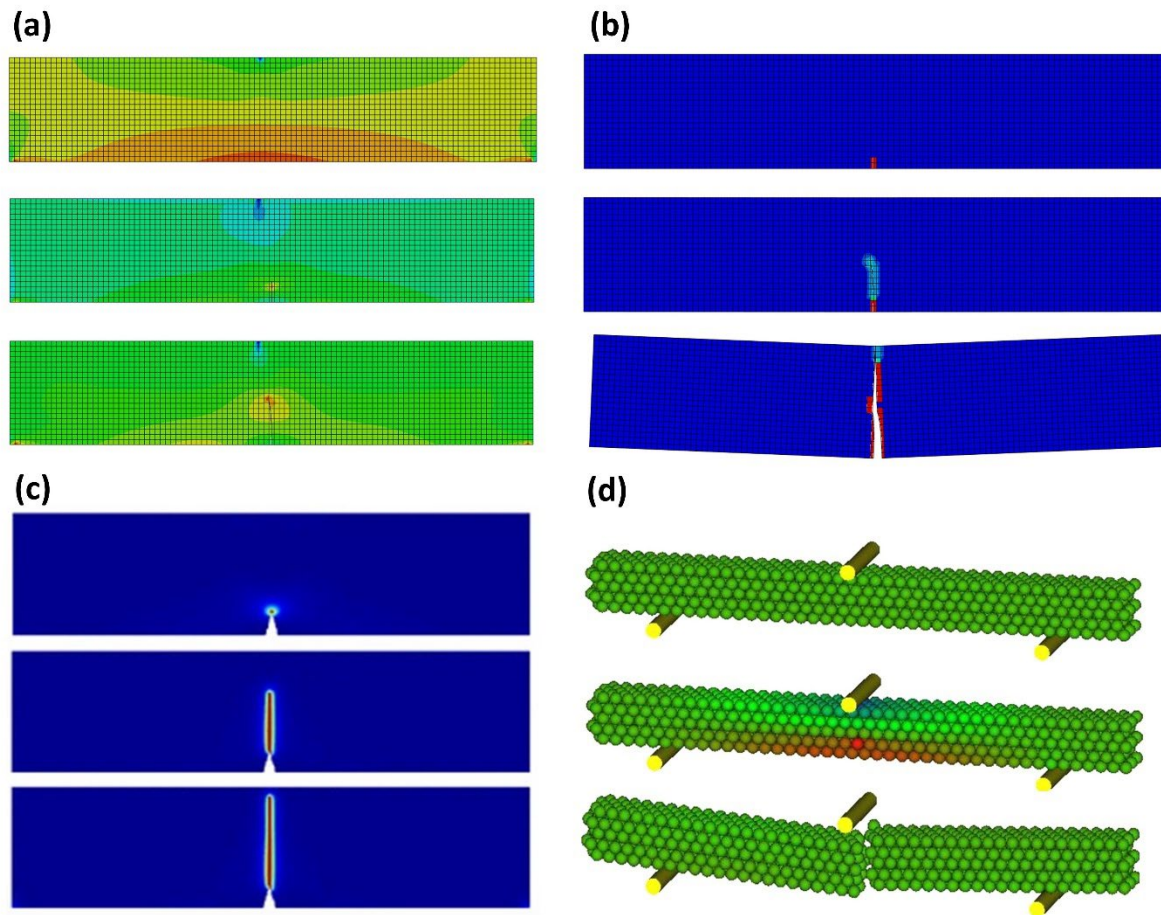


Figure 2.3: A benchmark engineering problem (3-Point bending test) simulated by different computational techniques. (a) The maximum principal stress contour from linear finite element analysis. (b) The crack path obtained by the eXtended Finite Element Method (XFEM). (c) The crack path obtained by the Phase-Field Method (PFM). (d) The crack path simulated by Discrete Element Method (DEM).

Table 2.2: A summary on different computational techniques for simulating the fracture behaviours in biostructures.

Modelling technique	Failure criteria	Implemented package	Software	Ref.
XFEM	Maximum principal stress	ABAQUS		[86, 101-110]
	Stress intensity factor	ANSYS		[111, 112]
	Strain energy release rate	COMSOL		[113, 114]
Phase-field	Strain energy release rate	ABAQUS		[115-118]
		COMSOL		[7, 119, 120]
CZM	Traction-separation law	ABAQUS		[121-123]
DEM	Force-displacement law	-		[124-126]

(a) eXtended Finite Element Method (XFEM)

XFEM, which is based on the partition of unity techniques, has proved to be one of the most effective and useful approaches to simulate the crack onset and propagation in brittle materials. It allows the insertion of a crack by introducing additional phantom nodes to the existing elements, in which the additional degrees of freedom enable to enrich the FE approximation. This enrichment in XFEM allows modelling discontinuities and singularities around the crack independent of the FE mesh adopted. To brief the mathematical background of XFEM, let all the nodes involved be denoted by set D , and the nodes around the cracking surface and tip are represented by the subset D_s and D_t , respectively. Thus, the approach for displacement calculation with crack modelling in XFEM can be expressed as,

$$\mathbf{u} = \sum_{j=1}^n N_j(x) [\mathbf{u}_j + H(x)\mathbf{a}_j + \sum_{\alpha=1}^{ne(j)} F_{\alpha}(x)\mathbf{b}_j^{\alpha}] \quad (2.1)$$

where N_j represents the conventional shape functions associated to node j , $\mathbf{u}_j$ stands for the standard nodal displacement, $H(x)$ is the Heaviside function, which is given as in Eq. (2.2). $\mathbf{a}_j$ denotes the additional degree of freedom associated with Heaviside function. $F_\alpha(x)$ is crack tip function. $\mathbf{b}_j$ stands for the extra degree of freedom accompanying with crack tip function, and $ne(j)$ represents the number of $F_\alpha(x)$ for node j .

$$H(x) = \begin{cases} 1, & \text{if } (\mathbf{x} - \mathbf{x}^*)\mathbf{n} \geq 0 \\ -1, & \text{otherwise} \end{cases} \quad (2.2)$$

where x is the arbitrary point near the crack face, x^* is the closet point to x , where is located on the crack surface. $\mathbf{n}$ is the outward unit vector normal to the crack at point x^* .

A key advantage of XFEM is that the mesh is not required to conform with the cracking geometry. Note that the Level Set Method (LSM) is a powerful numerical technique for simulating and analysing interface motion, which is used in XFEM to model arbitrary crack growth without remeshing. Two almost-orthogonal functions, namely $\phi(\mathbf{x}, t)$ and $\psi(\mathbf{x}, t)$, are utilized to define the geometry of the crack surface. The first function, $\phi(\mathbf{x}, t)$, defines the crack surface where $\mathbf{x}$ and t denote the point in space and time domain, respectively. The second function, $\psi(\mathbf{x}, t)$, is used to construct the orthogonal surface, so that the intersection of the two surfaces gives the crack front. This method does not require the explicit representation of the boundaries or interfaces because they are defined purely by the nodal data. Two signed distance functions per node are generally needed to describe a crack surface.

(b) Phase field method (PFM)

Phase field method which emerged as a nonlocal diffusive approach has proved effective for modelling brittle and ductile crack propagation. The key idea of the phase field fracture

modelling method is that discrete crack surfaces are assumed to be not sharp but to be interpreted as smeared or diffusive damage. In phase field approaches, the internal discontinuity of interfaces is modelled in terms of a continuous phase field variable ranging from 0 to 1, which represents sharp cracks by multiple physical phases through a smooth transition. The physical meaning of the phase field variable d can be given as in Eq. (2.3),

$$\begin{cases} d = 1, & \text{if the material is fully broken} \\ 0 < d < 1, & \text{if the material is diffusively damaged} \\ d = 0, & \text{if the material is undamaged,} \end{cases} \quad (2.3)$$

where $d = 0$ denotes the undamaged material, while $d = 1$ indicates the fully broken material. The material in the smooth transition area is associated with $0 < d < 1$, referred as crack field.

Phase field method originated from the variational formulation, and its regularised form of brittle fracture was established by Francfort, Marigo and Bourdin [127, 128]. The major advantage of phase field method is its ease of numerical implementation, as complex algorithms are no more required to track cracked surfaces in contrast to many other discrete models. It enables to mimic the cracks branching and intersection, which may not be performed in the XFEM easily. The damage in phase field models is based on the minimisation of a potential energy function during crack propagation processes.

The key idea of phase field models is to introduce a density function of crack surface with respect to phase field variable d and its gradient ∇d . First, the fracture energy release rate together with the crack surface density function is employed to calculate fracture energy. Second, a monolithically degradable strain energy function is defined or derived based on stress and phase field variable d . Finally, the variations of external work and the potential

energy function composed of the fracture energy and the degradable strain energy are performed to formulate governing equations within a phase field framework.

(c) Cohesive zone models

Cohesive models were first formulated by Bareblatt and Dugdale, who introduced finite nonlinear cohesive tractions in front of an existing crack as a means to overcome the stress singularity in the crack tip [129]. To date, the cohesive zone models (CZMs) have been widely used for numerical simulation of a fracture process. Cohesive zones represent the surfaces of discontinuities where displacements jump. A specific constitutive law relating the displacement jumps and proper tractions defines the cohesive zone model, and it is in contrast to the traditional approach of fracture mechanics where stress analysis is separated from a description of the actual process of material failure.

For a brittle or quasi-brittle material, Hillerborg et al. [130] suggested a linear decreasing law to describe the relationship between the normalized traction and separation. Based on this law, a number of researchers investigated the quasi-brittle fracture processes in various materials. For example, Elias and Le [123] proposed a cyclic cohesive zone model to simulate the mode-I crack growth in quasi-brittle structures under compressive cyclic loading. Zhang and Paulino [122] investigated the dynamic failure process in homogeneous and functionally graded materials (FGMs). The details of the traction-separation model will be discussed further in Section 2.2.3.

(d) Discrete element method

The discrete element method (DEM), originally proposed by Cundall and Strack in the context of rock mechanics, is a numerical technique that models the interaction between

individual particles and boundaries to predict bulk solid behaviour [131]. A specified force-displacement law was employed to determine the contact forces among particles from the overlapping and relative movements. DEM allows particles to be bonded together at contact and to be separated under external forces. Not only can it simulate the motion of individual particles, but also the behaviour of bulk material formed by assembling many particles through bonds at contact. The significant advantage of DEM is the capacity to explicitly model particle scale; thus, DEM allows for the simulation of microstructure and study of the micro/meso-level phenomena on the macroscopic fracture behaviour of ceramic materials. Some commercial DEM codes have been developed, such as Particle Flow Code (PFC), Discontinuous Deformation Analysis (DDA), Distinct Lattice Spring Model (DLSM), and Universal Distinct Element Code (UDEC). These simulation codes can effectively mimic the evolution of contact forces, broken contacts, and crack displacements within the DEM framework.

(e) Meshfree method

Despite the significant achievement in the Finite Element Method, mesh generation and element-based interpolation bring formidable difficulties in analyzing fracture process. To address this challenge, several meshfree methods have been developed attempting to avoid the burdensome task of meshing and remeshing in FEM. One positive feature of these methods is the resulting smooth stresses which can be obtained for high-stress gradients around crack tips thus requiring less effort in post-processing as compared with the traditional FEA framework. Meshless methods, such as Element Free Galerkin Method (EFGM), Reproducing Kernel Particle Method (RKPM), and Radial Point Interpolation

Method (RPIM), have successfully used for crack modeling, dynamic fracture modeling, damage mechanics.

2.2.2 Fracture damage models

When ceramic materials are used in load-bearing applications, structural failure is a major concern. Conventional fracture analysis normally consists of three main steps. First, a constitutive equation, which forms the basis for modelling, is either chosen in the commercial FE software package or defined by user-subroutine using experimental data. Second, FEA program calculates the displacement and strain-stress of the system. Third, the FEA results are used to evaluate the fracture strength according to various failure criteria. According to the literature, the fracture failure of load-bearing prostheses can be caused by either overloading fracture or fatigue failure, in which the mechanical stresses for damage could be considerably lower than the material strength. The details of failure model will be discussed in this section.

2.2.2.1 Static failure criteria

Static failure criteria are often used to examine whether the overload fracture takes place when a structure is under a static/quasi-static loading [132]. The brittle materials are prone to fracture under tensile loadings rather than compressive loadings, thus Maximum Principal Stress (MPS) is one of the most crucial indicators that associate with the fracture behaviours in ceramic materials [106]. In addition, with the development of hybrid and/or composite materials, polymers offer great potential to reduce the brittleness of pure ceramic materials thereby enhancing the toughness [19]. For those materials, von Mises stress theory is extensively adopted to predict the failure by considering yield strength.

(a) Maximum principal stress (MPS) criterion

The maximum principal stress is one of the most commonly used criteria in the brittle materials, which states that the fracture could occur when the maximum principal stress in the material exceeds the local strength. The MPS criterion can be expressed as,

$$f = \left\{ \frac{\langle \sigma_{max} \rangle}{\sigma_{max}^0} \right\} \quad (2.4)$$

where σ_{max}^0 represents the maximum allowable stress, also named as ultimate tensile strength; the symbol $\langle \rangle$ represents the Macaulay bracket which signifies that a purely compressive stress state may not initiate damage. Damage is assumed to initiate when the maximum principal stress ratio, f , reaches a value of 1.

(b) von Mises stress (VMS) criterion

To consider the shear stresses and compressive stress, von Mises stress criterion is widely used to predict the strength of ceramic composite materials. As failure occurs when von Mises stress values exceed the yield strength, von Mises stress criterion is important for interpreting the stresses occurring in the relatively ductile materials, such as polymer-infiltrated ceramic network [133]. The von Mises stress (σ_{vms}) represents the distortion energy in the material as expressed as,

$$\sigma_{vms} = \sqrt{\frac{1}{2} \left[(\sigma_{xx} - \sigma_{yy})^2 + (\sigma_{yy} - \sigma_{zz})^2 + (\sigma_{zz} - \sigma_{xx})^2 \right] + 3(\tau_{xy}^2 + \tau_{yz}^2 + \tau_{zx}^2)} \quad (2.5)$$

where σ_{xx} , σ_{yy} , and σ_{zz} are the normal stresses, and τ_{xy} , τ_{yz} , and τ_{zx} are the shear stresses.

(c) Strain energy release rate criterion

The energy-based damage evolution criterion was adopted in a number of studies to mimic both crack formation and subsequent propagation [115, 116]. The strain energy release rate, $G(J/m^2)$, is the energy dissipated per unit area of a newly created crack surface area. Due to the absence of a well-defined straight crack, the critical stress intensity factors, $K_{I,II,III}$, may not be easily determined following the conventional concepts of fracture mechanics. To overcome this, strain energy release rate which can be calculated based on J integral, has been introduced in the simulation programs. As the Mode-I fracture is normally dominant in the brittle and quasi-brittle materials, the strain energy release rate can be formulated in relation to fracture toughness as,

$$G_I = \frac{K_I^2}{E} \quad (2.6)$$

where K_I is Mode-I stress intensity factor, E is Young's modulus of material.

Therefore, the energy release rate criterion can be expressed as,

$$K_I \geq K_{IC} \quad (2.7)$$

where K_{IC} is fracture toughness of Mode I.

2.2.2.2 Fatigue failure criteria

Apparent from the static fracture, fatigue failure due to cyclic loading is another common and major concern in prosthetic devices. A number of researchers made great efforts to estimate the fatigue life by using various computational methods. FEA is one of the most representative approaches for determining the stress level and can be used to predict fatigue

life based upon different fatigue models. This section summarises some common fatigue models used in the numerical methods which have gained widespread acceptance.

(a) Stress method

Stress-based fatigue models are generally related to high-cycle fatigue, in which a major part of the material behaves elastically [134]. Fatigue life is estimated by using an empirical S - N curve in accordance with various failure criteria as the basis. The S - N curve can be established for fatigue tests of material, which is used to predict the number of cycles to failure, as [134]

$$\Delta\sigma = \sigma_f (N_f)^B \quad (2.8)$$

where $\Delta\sigma$ is the applied stress amplitude, σ_f is failure stress, N_f is the number of fatigue cycles, B is the fitting parameter determined by experiments.

In order to assess the fatigue endurance limits, some researchers adopted various criteria, including Goodman, Morrow, and Soderberg, to determine the safe region under the cyclic loading [135]. These three criteria use different material strength, yielding strength for Soderberg, ultimate tensile strength for Goodman, and true fracture strength for Morrow.

(b) Strain method

A number of researchers proposed to adopt different strain-based models to predict fatigue failure, e.g., Coffin-Manson [136], Basquin and Solomon [137]. The Coffin-Manson model is perhaps the best known and most widely used approach today. The number of cycles to failure, N_f , is dependent on the plastic strain amplitude, $\Delta\varepsilon_p$, the fatigue ductility

coefficient, ε'_f and fatigue ductility exponent, c [136]. The relationship among these variables is expressed in Eq. (2.9),

$$\Delta\varepsilon_p = \varepsilon'_f N_f^c \quad (2.9)$$

To take the elastic deformation into consideration, the Coffin-Manson model is usually combined with Basquin's equation [137]. The resultant equation is known as the total strain model formulated as

$$\Delta\varepsilon = \sigma'_f E N_f^b + \varepsilon'_f N_f^c \quad (2.10)$$

where $\Delta\varepsilon$ is the strain range, σ'_f is the fatigue strength coefficient, E is the elastic modulus, ε'_f is the fatigue ductility, b is the fatigue strength exponent, and c is the fatigue ductility exponent.

Solomon's low cycle fatigue model relating the plastic shear strain to fatigue life cycles is shown in Eq. (2.11) [135],

$$\Delta\gamma_p (N_p)^\alpha = \theta \quad (2.11)$$

where $\Delta\gamma_p$ is the plastic shear strain range, N_p is the number of cycles to failure, θ is the inverse of the fatigue ductility coefficient, and α is a material exponent.

(c) Strain energy method

Energy-based fatigue life estimation attempts to consider the hysteresis information into fatigue modelling. The fatigue criterion is based on the hysteresis energy, which can be obtained from the volume-weighted stress-strain history. Fatigue energy is typically

calculated using some correlation to the energy under the stress-strain hysteresis loop. The fatigue life can be calculated according to an energy-based fatigue failure criterion as shown in Eq. (2.12) [138, 139],

$$N_f = A(\Delta W)^B \quad (2.12)$$

where N_f is the number of cycles to failure, ΔW is the hysteresis strain energy per cycle, A and B are material constants, which can be determined via a fitting exercise correlating with the corresponding experimental data.

Compared to the strain-based counterparts, energy-based fatigue models enable to predict the accumulated energy required to initiate a crack, rather than the ultimate fatigue failure. The benefit of energy-based fatigue model is to capture testing conditions with better accuracy. For complex waveform stress-strain hysteresis curves, the energy-based fatigue models are better for simulating the accumulated damage.

2.2.2.2 Debonding failure

The damage in cohesive interface is defined via traction-separation criterion. The traction-separation model used herein includes a linear elastic phase and a subsequent damage progression phase. The nominal traction stress vector, $\mathbf{t}$, can be formulated as

$$\mathbf{t} = \begin{Bmatrix} t_n \\ t_s \\ t_t \end{Bmatrix} = \begin{bmatrix} E_{nn} & 0 & 0 \\ 0 & E_{ss} & 0 \\ 0 & 0 & E_{tt} \end{bmatrix} \cdot \begin{Bmatrix} \varepsilon_n \\ \varepsilon_s \\ \varepsilon_t \end{Bmatrix} \quad (2.13)$$

where t_n is the normal component of the stress traction vector and t_s and t_t are the two shear traction components, respectively. E_{nn} , E_{ss} , and E_{tt} are the elastic modulus in each

respective direction. ε_n , ε_s , and ε_t are the elemental strains related to the normal and shear stresses.

To assess the risk of debonding, traction-separation law was adopted by many researchers. The tensile and shear stresses are commonly recognized as a trigger to initiate the crack [140, 141]. In literature, there are two main frameworks to model the adhesion failure, namely maximum nominal stress criterion and quadratic nominal stress criterion, which can be shown by Eq. (2.14) and Eq. (2.15) respectively,

$$\max \left\{ \frac{\langle t_n \rangle}{t_n^0}, \frac{t_s}{t_s^0}, \frac{t_t}{t_t^0} \right\} = 1 \quad (2.14)$$

$$\left(\frac{\langle t_n \rangle}{t_n^0} \right)^2 + \left(\frac{t_s}{t_s^0} \right)^2 + \left(\frac{t_t}{t_t^0} \right)^2 = 1 \quad (2.15)$$

where t_n^0 , t_s^0 , and t_t^0 represent the interface strength in the normal and two shear directions, respectively. The symbol $\langle \rangle$ represents the Macaulay bracket implying that a purely compressive stress state does not initiate damage. Damage is assumed to initiate when the maximum nominal stress ratio or a total quadratic nominal stress ratio reaches a value of 1.

2.3 Dental applications

The growing demand of aesthetics has led to the development of metal-free dental restorations without metallic components [142]. Dental ceramics present numerous favourable features, including biocompatibility and excellent potential to simulate the optical characteristics of natural teeth [142]. However, the evaluation of clinical survival rates of posterior all-ceramic crowns and fixed dental prostheses (FDPs) reveals the vulnerability of those systems to various failure modes [143]. Therefore, many clinical trials and experimental tests have been performed to evaluate and enhance the fracture strength of all-ceramic restorations, including structural design, optimising tooth preparation, material selection, etc. For a comparative purpose, the material properties of various ceramic materials used in dental applications are summarised in Table 2.3.

Table 2.3: Summary on material properties for ceramic materials used in dental application.

	Young's Modulus, E (MPa)	Poisson's Ratio ν	Tensile Stress σ_{TS} (MPa)	Fracture Toughness K_{IC} (MPa·m ^{1/2})	Refs.
Lithium disilicate (LDS)	95,000- 120,000	0.22-0.25	210-376	2.04-2.27	[13, 32, 95, 106, 144- 146]
Yttria stabilized tetragonal zirconia (Y- TZP)	200,000- 217,450	0.24-0.32	742-1,200	4.2-6.3	[41, 79, 96, 106, 147- 150]
Hybrid polymer- infiltrated ceramic network material (PIC)	30,000- 37,800	0.23-0.28	135.8-148	1.2	[54, 65, 79, 106, 144]
Feldspar ceramic (FC)	48,700-	0.22-0.23	122	1.23-1.25	[96, 106,

	72,000				144, 145]
Aluminum oxide-reinforced porcelain	120,000	0.27	300	-	[53]
Leucite-free glass ceramic (Veneering porcelain)	60,000-70,000	0.19-0.3	61-140	0.71-0.75	[52, 53, 92]
Leucite-reinforced ceramic	62,300-75,700	0.23-0.31	65-112	0.81-1.22	[32, 99, 100, 151]
Lithium disilicate reinforced glass	65,000-98,000	0.22-0.3	100-160	1.06-1.94	[95, 99, 152, 153]
Borosilicate glass	62,500	0.19	83.2	0.77	[20]

2.3.1 Crowns

Dental crowns (as shown in Figure 2.4 (a) and (b)) are widely used to restore a broken or decayed tooth when too much of the original tooth tissue is missing or has to be removed. Nevertheless, fractures are one of the main problems reported in clinical follow-up studies, as shown in Figure 2.4 (c). Numerical studies have been recognized as a powerful tool to investigate the fracture behaviour of the crowns. Due to the challenges in modelling the complex crown geometries, some earlier studies performed the simulations based on the 2D models or simplified crown models (e.g., Figure 2.4 (d)). With recent advancements in computational power, it has become possible to create 3D models of dental prostheses based on CT scan images using image reconstruction techniques [125, 180]. These advancements allow researchers to explore the effects of detailed geometrical features on the performance of dental prostheses, as shown in Figure 2.4 (e).

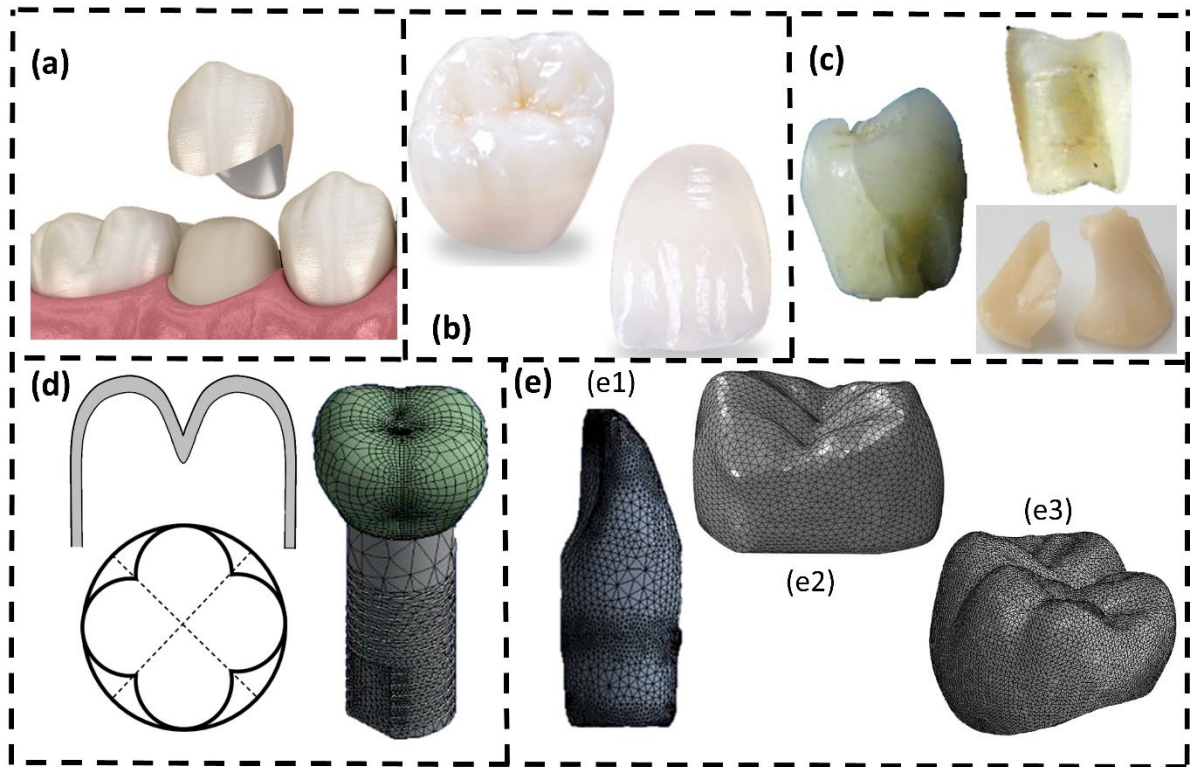


Figure 2.4: (a) The demonstration of dental crown. (b) Representative models for ceramic molar and incisor crowns. (c) Typical fracture patterns in premolar and incisor [181, 182]. (d) Simplified crown model [33, 122]. (e) Represent the FE models for different teeth [183] [125]; (f1) incisor crown-tooth model. (f2) premolar crown model. (f3) molar crown model.

While core-veneered and monolithic dental crowns have become a popular all-ceramic restoration of choice attributable to their excellent chemical durability, biological compatibility and aesthetic appearance, fracture remains one of the main issues reported for ceramic restorations in clinical practice. In general, the success of ceramic restorations depends on several factors, such as material properties, restorative design, and cementation bonding. These factors will be reviewed in the following sections and are summarised in Table 2.4 for clarity.

Table 2.4: Summary of numerical studies on fracture predictions/investigations of dental crowns made of bio-ceramics.

Research aims	Loading types	Failure criteria	Contact conditions	Refs.
Design optimisation	Static loading	MPS	Perfectly bonded	[11, 36, 41, 47, 53, 83, 92, 93]
				[3, 103, 154, 155]
			-	[58, 156, 157]
	Cyclic loading	Stress based fatigue criterion	Perfectly bonded	[46, 149, 158]
		Strain based fatigue criterion	Perfectly bonded	[159, 160]
				[31, 65]
Bonding interface	Static loading	MPS	Perfectly bonded	[57, 150, 152, 161, 162]
			Frictional contact (0.1)	[163]
			Frictional contact (0.3)	[164, 165]
	Cyclic loading	Strain based fatigue criterion	Frictional contact (0.45)	[97]
		Stress-based fatigue criterion	Frictionless	[20]
			Element-depended	[55, 56, 96]

(CZM)				
Material selection	Static loading	MPS	Perfectly bonded	[12, 13, 21]
			-	[59, 106, 147]
			-	[32, 52, 144]
	Cyclic loading	von Mises stress	Perfectly bonded	[146]
			-	[21, 40]
			-	[42, 48, 95]
Thermal induced loading	Transient loading	Stress based fatigue criterion	Perfectly bonded	[79, 85, 166]
			-	[167]
			-	[86, 94]
	Transient loading	MPS	Perfect bonded	[14, 90, 148,
			-	168, 169] [1, 4-6, 87, 91, 170]

2.3.1.1 Core-veneering crown

When aesthetics is of utmost importance, bi-layered ceramic system is one of the most commonly used dental crowns, which have an inner layer of high-strength core ceramic and an outer layer of more aesthetic and transparent veneering ceramic, as shown in Figure 2.5 (a) [86]. Compared to monolithic restorations, bi-layered all-ceramic crowns provide outstanding aesthetic results and have been more commonly used in the anterior region of the mouth, where the aesthetic appearance is more critical [171]. Despite the advantages, the relatively low fracture resistance of bi-layered structures is the main concern in practice which needs to be improved by optimising the material combination, geometrical design, etc. [172, 173]

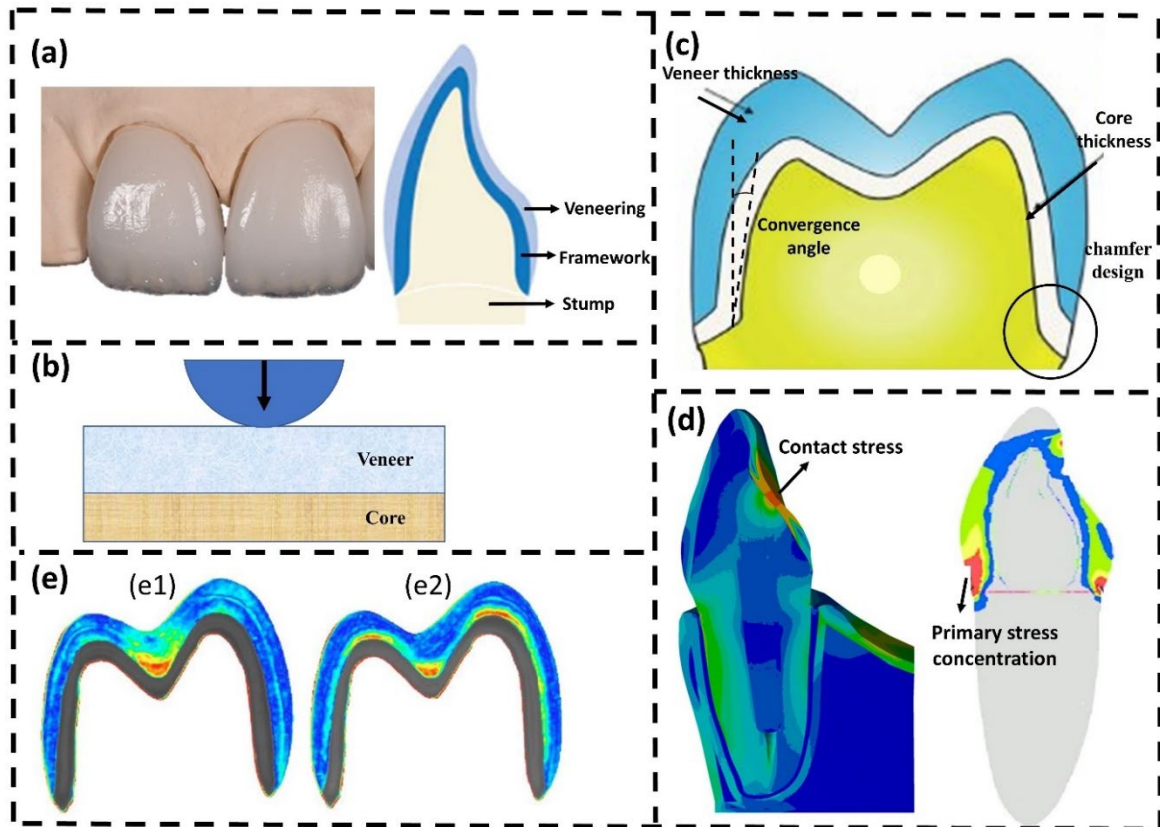


Figure 2.5: (a) The demonstration of veneered dental crown. (b) Schematic diagram of Hertzian contact testing in a bi-layered planar sample. (c) Design parameters in the core-veneering crown [171]. (d) Representative stress distribution in the incisor core-veneered crown [172]. (e) Representative thermal residual stress distributions due to the mismatch between zirconia infrastructure and the veneer porcelain; (e1) fast cooling rate; (e2) slow cooling rate [173].

(a) Effect of material selection

To match the natural teeth accurately in terms of colour and translucency, dental porcelain is the most commonly used material to fabricate the veneer layer which is fused to

the zirconia or alumina based ceramic cores. To evaluate the fracture properties of bi-layered configurations, some researchers conducted Hertzian contact testing of bi-layered planar samples (as shown in Figure 2.5 (b)) with dental porcelain on the top and core material on the bottom [174]. The main advantage of this testing model is that its relatively simple geometry enables to reduce the noise factors, hence allowing researchers to focus on the effect of material properties. The results showed radial cracks played a crucial role in causing bulk fracture, which could be responsible for the failure of in-service crowns [13]. In order to reduce the radial cracks, Lawn et al. [52] suggested a strong and tough core material, such as Y-TZP zirconia, should be used to improve the performance of an all-ceramic crown. With the introduction of such stronger core materials, the cores are sufficiently strong to withstand a long-lasting lifespan; however, such core materials do not always result in lower stresses in the veneering porcelain. To minimise the fracture risks in veneering porcelain, Al-Maqtari et al. [12] and Mahmoudi et al. [21] utilise the functional-graded material (FDM) to replace the conventional single ceramic cores. The results showed that FDM not only decreased the stress magnitude in the ceramic core, but also reduced the shear stress at the bonding interface.

(b) Effect of geometrical designs

Optimising core and veneer designs may contribute to balancing the competing requirements including adequate fracture strength, aesthetics, and extent of removal of tooth tissue. However, the effects of geometrical parameters are inconsistent, and the clinical relevance is uncertain from the open literature, therefore, the optimal design for the veered crowns is not definitively established. Design parameters of core-veneering crowns consist of two aspects, tooth preparation and occlusal design [85]. Many efforts have been made to

evaluate the effect of these two groups on fracture strength of bi-layered crowns. According to the literature, as demonstrated in Figure 2.5 (c), tooth preparation mainly includes the chamfer design, tooth convergence angle, axial wall height and core/veneer thickness. In the pursuit of optimizing incisor crown designs, stress magnitude is considered as a crucial design requirement as it closely correlates with fracture susceptibility. Figure 2.5 (d) demonstrates that under occlusal loading, the stress concentration primarily occurs in the chamfer region. For example, Li et al. [11] studied the effect of incisor chamfer on the mechanical behaviour of veneers and found that the palatal chamfer design for porcelain laminate veneers had better tolerance to stress. Both De Jager et al. [53] and Zarone [83] suggested that a chamfer with collar preparation is beneficial to the veneering porcelain. Corazza et al. [149] investigated the influence of the convergence angle of tooth preparation on the fracture load of veneered restorations, and the results showed that 20° of total occlusal convergence angle had the highest load capacity to fracture in their models. Axial wall height is another tooth preparation parameter. Rekow et al. [92] suggested that the stress concentration area is an important indicator of crack initiation sites, and they found that the magnitude of stress concentration at the margin of the core was directly related to the axial wall height of the crown periphery. The numerical results revealed that the stress values decreased with the increase in axial wall height. Moreover, Costa et al. [174] studied the effect of core/veneer thickness ratio on the stress distribution of the veneered crown and they suggested that a thicker veneer can result in a more desirable stress distribution which indicates a higher fracture resistance. Rafferty et al. [93] studied the interactive effect of core thickness, cement thickness and wall height reduction on the tensile stress magnitude in the veneer layer.

In terms of the occlusal design, Hu et al. [36] utilized computational tools to optimise the coping designs of all-ceramic crowns; and found that the modified coping without veneer coverage on the lingual side exhibited the minimum fracture risk under the occlusal loading. Shahrabaf et al. [154] and Anami et al. [41] found that a flat occlusal design showed a more benign stress distribution in ceramic crowns compared to an anatomic design. Motta et al. [31] revealed that when a flat occlusal reduction already exists, the substructure needs to reproduce a correct anatomic form for a uniform thickness of the veneering porcelain.

(c) Effect of bonding interface:

Literature studies identify that bonding characteristic of interface play an important role in the structural integrity and mechanical strength of ceramic restoration. For example, Kanat-Erturk et al. [96] evaluated the effects of veneering techniques on the strength of zirconia framework. Their results indicated that layering or pressing may reduce ceramic chipping, but the over-cemented file-splitting method did not seem to prevent this failure. The effect of cement stiffness on the stress state of the ceramic-tooth system was evaluated by Shahrabaf et al. [154] and they found that the cement stiffness had a more profound effect on the stress distribution in the remaining tooth, rather than the crown. For the same cement, Rezende et al. [150] observed that a thicker cement space led to a higher stress concentration in bi-layered ceramic crowns. The non-uniform cement layer could give rise to a poor bonding interface between veneering porcelain and those strong ceramic cores, further compromising the strength of overall ceramic structures. Rocha et al. [164, 174] and Lazari et al. [165] found that an incomplete bond can cause a higher tensile stress concentration in the ceramic veneer compared with a perfect bonding condition.

(d) Thermal stress:

Bilayered prosthetic structures were often made through sintering process, in which thermal-induced stress from rapid cooling of the poor thermally conducting zirconia and porcelain materials is one of the major concerns in veneered dental restoration [4]. As shown in Figure 2.5 (e), Fabris et al. [4] simulated the residual stress map of veneered crowns under both fast and slow cooling rate. They found that the inner curved interface of crown had the peak stress concentration. According to the literature, thermal expansion mismatch and cooling rate-induced tempering stress are two important factors leading to the veneered crown cracking [176]. Benetti et al. [90] and Bonfante et al. [94, 148] studied the thermomechanical stress in monolithic ceramic crowns and ceramic veneer layered crowns. It was shown that the severe tempering stresses within the zirconia-porcelain system can be caused by the rapid cooling rate, and such stresses may result in unstable chipping cracks. Similarly, Zhang et al. [86, 170] and Kim [87] suggested that fast cooling can directly lead to thermal fracture in the ceramic structures. Furthermore, Tanaka et al. [91] reported that extremely slow cooling rate could have a deleterious effect on the laminated ceramic materials compared to the recommended rates by the manufacturer.

To reduce the thermal induced stresses, functionally graded materials (FGM) have been introduced to replace conventional veneer materials. Henriques et al. [5, 6] carried out a series of studies to examine the distribution of residual thermal stresses arising in the functionally graded material (FGM) of dental restorations after a cooling process. The results indicated that the FGM interlayer could significantly improve the stress profiles and reduce the stress magnitude compared to the conventional material (up to 70% at specific locations, e.g., interlayer interface). Besides FGM, researchers also optimized the structural parameters to minimise the fracture risk caused by thermal stress. For instance, Celebi et al. [14] suggested that butt joint preparation could reduce the stress values compared to the palatal

chamfer due to a larger adhesive surface area. Zhang et al. [86, 170] explored the effects of layer thickness on the fracture resistance of bi-layered ceramic restorations. It was found that the greater the thickness ratio of zirconia to veneer layer, the smaller the thermal residual stress and the lower the fracture risk.

2.3.1.2 Monolithic crowns

The clinical data suggested that adhesive fracture and chipping are major failure modes for bilayer dental crowns. While, in general, feldspathic or glass-veneer ceramic crowns have been fairly successful in the anterior region with a reasonable survival rate up to 10 years, this was not the case for posterior crowns. To accommodate the relatively high occlusal forces, monolithic crowns have been introduced as alternatives to porcelain veneered crowns to increase fracture strength and reduce the risk of adhesive fractures. As shown in Figure 2.6 (a), Fathy et al. [46] compared the principal stress distribution for fully milled and layered crowns, and the results showed that the porcelain veneer experienced a higher deformation than the monolithic crown and transferred lower energy to the core substructure. Therefore, the layered crown might have a higher probability of veneer chipping. Zhang et al. [13] also suggested that monolithic crowns were able to sustain high bite forces.

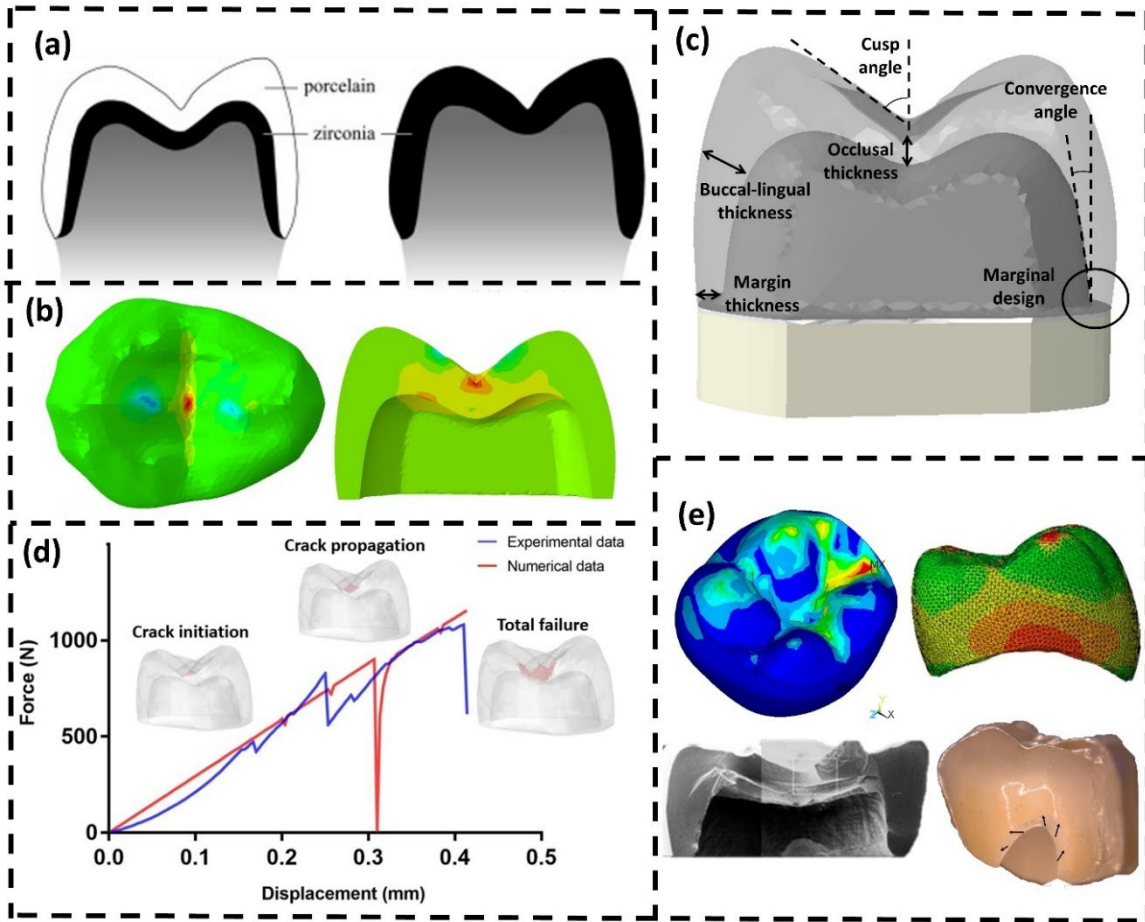


Figure 2.6: Numerical simulation results for dental crowns. (a) Schematic of monolithic dental crown. (b) Maximum principal stress distribution in a premolar crown. (c) Design parameters of monolithic crowns. (d) Correlation of force-displacement curve obtained from the simulation and laboratory test as well as the corresponding crack pattern in a premolar crown. (e) The representative maximum principal stress distributions in molar crowns, and the corresponding crack patterns [159, 161, 175].

(a) Effects of material selection:

Material properties play a primary role in determining the mechanical strengths of the prosthetic structures. Dejak et al. [40] compared the strength of thin-walled molar crowns made of various materials and concluded that equivalent stress decreased with the increasing Young's modulus of the materials. Shahmoradi et al. [106] conducted a more specific comparison of the CAD/CAM dental ceramics, lithium disilicate, feldspar ceramic, zirconia, hybrid resin ceramic and hybrid polymer-infiltrated ceramic. The results indicated that the zirconia crowns exhibited the highest fracture resistance of these candidate ceramic materials. A number of researchers [79, 166, 167] also compared the fatigue life of molar crowns made by all-ceramic CAD/CAM materials, and it was found that the zirconia also exhibits the longest lifespan compared to lithium disilicate, etc. Bataineh et al. [79] investigated the effect of chemical compositions, treatment, and post-processing techniques. They found that IPS e.max ZirCAD sintered at 1450°C had superior fatigue resistance.

(b) Effect of geometrical designs:

In terms of the premolar crown, the stress is mainly concentrated in the occlusal fissure region (Figure 2.6 (b)), which is a primary concern for the crown stability. To enhance the fracture resistance of crowns, a number of researchers have optimised crown geometry, including internal parameters (preparation height, shoulder margin, and convergence angle) and external parameters (crown thickness, cusp angle, and occlusal notch design), as demonstrated in Figure 2.6 (c). For example, Juloski et al. [47] and Maghami et al. [156] found a higher preparation height generated a more favourable stress distribution in the ceramic component in the restored tooth. Miura et al. [58] revealed that the rounded shoulder margin and deep chamfer margin could provide an optimal geometry to minimise occlusal

stress. Zhang et al. [103] also suggested that crowns with thicker margins and smaller convergence angles would improve fracture resistance. Regarding the external parameters, Dal Piva et al. [159] and Machry et al. [160] identified that a higher stress concentration was presented in the thinner crowns. Borges et al. [155] found that the reduced slope of cusp angulation could reduce the stress concentration and increase the fracture load. Shahmoradi et al. [106] investigated the collective effect of notch design, cusp angle and crown thickness, and they found that the most conservative design is the rounded notch with around 1.05 mm crown thickness and 60° cusp angle and the corresponding experimental validation for the numerical simulation is shown in Figure 2.6 (d). The stress distribution in molar crowns is notably more intricate compared to premolars due to the complex occlusal morphology. Besides occlusal splitting fractures, there is an additional concern regarding marginal cracking, as shown in the Figure 2.6 (e), Øilo et al. [175] found that the hoop-stress is the main cause for such cervical cracking.

(c) Effect of bonding interface

Besides occlusal surface cracking, the bonding interface is one of the most typical fracture location origins [20]. It is well known that the cement layer plays an essential role in the fracture resistance of the all-ceramic crown system, because it is critical to maintain the average principal tensile stress between the crown and tooth [97, 163]. For example, Dong et al. [57] and Ha [162] evaluated the influence of various cement stiffness on the stress distribution in monolithic ceramic crowns. They suggested that the resin cement was recommended for the luting agent due to the proper elastic modulus. For the similar cement materials, Liu et al. [152] and Ha et al. [161] found that an optimal cement thickness (0.09-0.1 mm) could reduce the stress level in ceramic crowns.

(d) Effect of occlusal loading concepts

The occlusal loadings on the crowns are always complex, therefore, the effect of occlusal loading locations on the stress distribution is another important research topic in the field of prosthetic dentistry. The common simulation-based loading scenarios are summarised in Figure 2.7. The loading ball-crown system has been widely adopted in the existing literature to simulate laboratory compression tests, as shown in Figure 2.7 (a). To mimic a more realistic in-vivo occlusal loading, Duan and Griggs [19] identified the stress distribution of the crown under occlusal loadings with different inclination angles, and they suggested that the lateral occlusal loading component could result in a more profound stress increase in the prosthesis (Figure 2.7 (b)). Some researchers argued that the loadings on the crowned tooth are induced by the contact from the opposite tooth, as shown in Figure 2.7 (c), thus, the forces are distributed uniformly on the surface of the crown [176]. Dejak et al. [40] simulated the closing phase of mastication by including the restored tooth, the bolus and the opposite tooth for a more realistic modelling of physiological loading conditions.

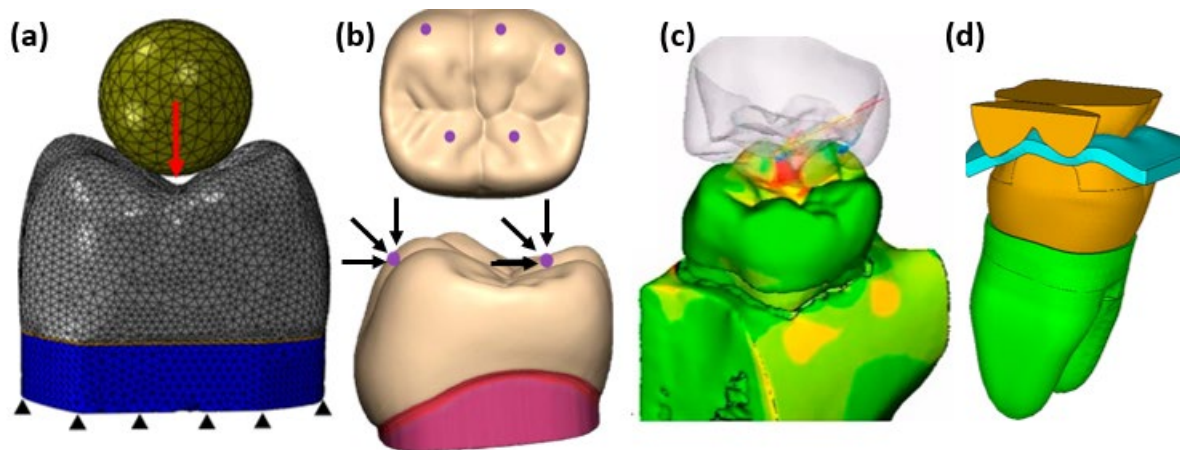


Figure 2.7: Various loading conditions on the dental crowns. (a) Laboratory compression test. The dental crown is under the compression from the loading ball. (b) The loads are directly applied to the occlusal surface based on the oral scan [161]. (c) The loadings are generated by the opposite tooth to mimic the tooth-tooth-contact [176]. (d) The loading condition for simulating the chewing process [40]. The third body was introduced to simulate the food chewing/biting process.

2.3.2 Fixed Partial Dentures (FPD)

In clinics, the replacement of missing teeth by using fixed partial dentures (FPDs) with full-ceramic frameworks has been a prevalent option, which is attached to adjacent teeth or dental implants permanently. It is more like a ‘bridge’ fixed on the ‘stages’, where the adjacent teeth or implants, called abutments, act as the stages to support the dental bridge. Three main components are structurally locked together in one FPD unit: pontic, retainer and connector (Figure 2.8 (a)). A pontic is an artificial tooth on an FPD that replaces the missing natural tooth and restores its function. A retainer is an important appliance that unites the

abutment teeth with the suspended portion of the bridge. Both intracoronal and extracoronal restorations can be used as retainers and are fixed by adhesion. A connector is another important appliance that unites the retainer(s) and pontic(s). When an occlusal force is applied to the pontic, it is transferred to the connector, retainer, and finally to the abutments and the surrounding bony structure by connecting the FPD and abutments together.

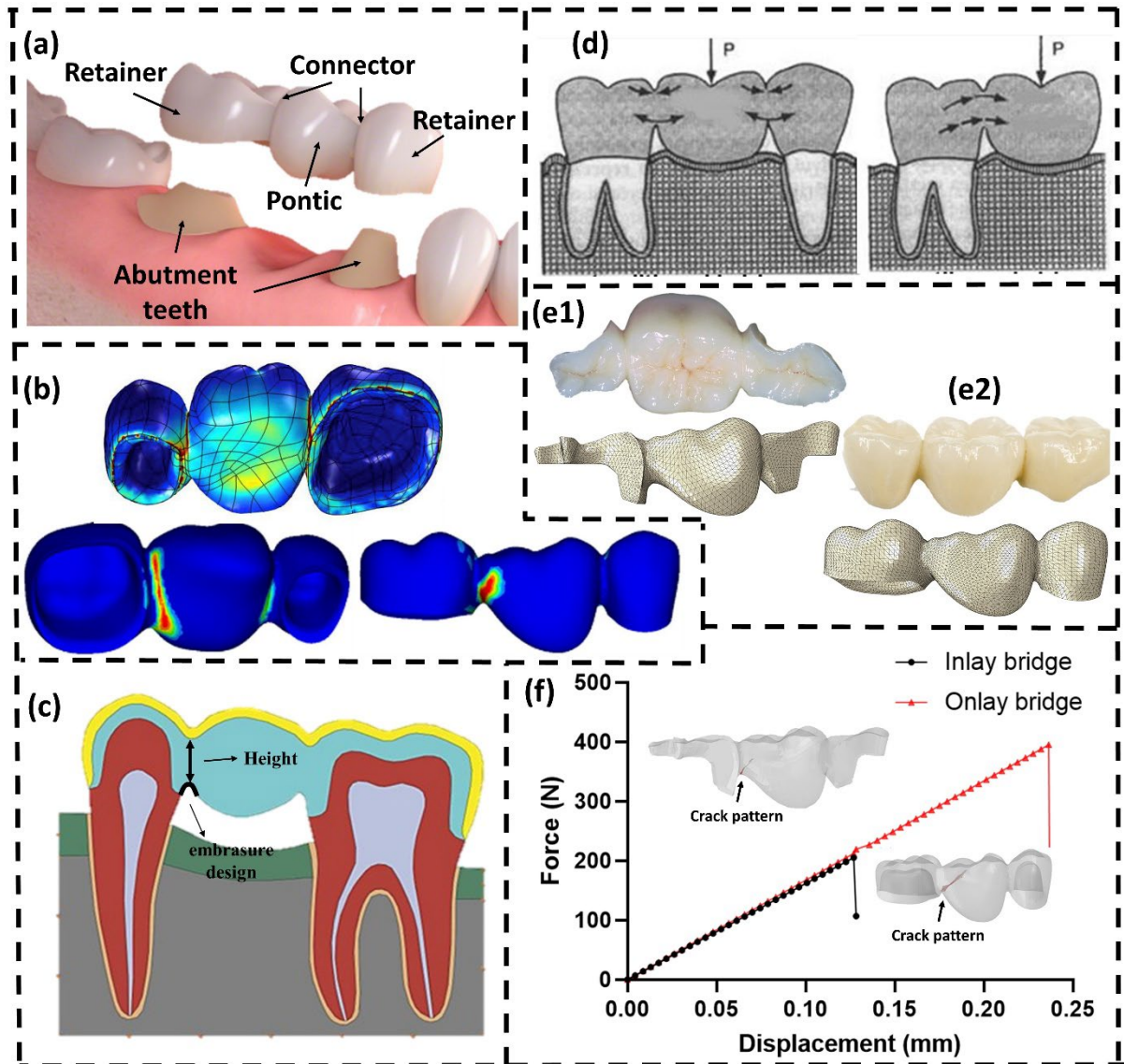


Figure 2.8: (a) The components of the fixed partial denture (FPD). (b) Representative stress distribution in the FPD and the crack path simulated by phase-field method [177]. (c) 2D

model for 3-unit FPD with design parameters. (d) Comparison between traditional 2-unit retainer FPD and single retainer (cantilever) FPD. (e1) 3D models for inlay FPD. (e2) 3D models for onlay FPD. (f) The force-displacement curves of inlay and onlay FPD with the simulated crack paths.

In vitro investigations, experimental and fractographic studies conducted on failed FPDs have revealed that the fracture origin and mode of failure of all-ceramic FPDs are substantially different from those of crowns. Kohorst et al. [178] introduced 3D FEA to examine the stress distribution in all-ceramic four-unit bridges. The results showcased the possibility of detecting the weakest points of dental restorations by virtual simulation of different loading conditions. In-silico finite element analysis demonstrated that during occlusal loading, the highest stress within FDPs was located at the connector areas rather than the occlusal surface, as shown in Figure 2.8 (b) [179-181]. More recently, Wu et al. [116, 117] proposed a relatively new phase-field model to simulate the crack propagation in FPDs. Table 2.5 summarises the FE studies on the structural strength and longevity of the FDPs.

Table 2.5: Summary of numerical studies on fracture predictions/investigations of FPDs made of bio-ceramics.

Research aims	Loading types	Failure criteria	Contact condition	Refs.
Design optimisation	Static loading	MPS	Perfectly bonded	[60, 102, 151]
		von Mises Stress	-	[182, 183]
		Fracture energy	Perfectly bonded	[64, 184]
	Cyclic loading	Stress based	Perfect bonded	[115-117]
		fatigue criterion		[185, 186]
Bonding	Static loading	MPS	Perfectly bonded	[187, 188]

interface				[179]
			Element dependent	[189, 190]
	Cyclic loading	Stress based fatigue criterion	Perfectly bonded	[143, 188]
Material selection	Static loading	MPS	Perfectly bonded	[9, 43, 69, 99, 191, 192]
			-	[63, 180]
	Cyclic loading	Strain based fatigue criterion	Perfectly bonded	[22, 24, 100]
		Stress based fatigue criterion	Perfectly bonded	[69, 84]
Thermal induced loading	Transient loading	MPS	Perfect bonded	[88, 89]

(a) Effect of material selection:

A number of researchers evaluated the von Mises stress and MPS in the restored molar tooth with different restorative materials; and they found that a lower Young's modulus can result in lower stress in the structure [24, 99, 193]. More specifically, lithium disilicate ceramic had a better performance in replacing the lost dentine and enamel than leucite and zirconia [66, 84]. Ma et al. [9] compared the load-bearing capacity of an occlusal bridge made of lithium disilicate and monolithic zirconia, and the results revealed that the loading capacity of minimally invasive lithium disilicate can exceed 70% of that of zirconia.

Concerning the bilayered structured FPDs, the more rigid core material can lead to less tensile stress concentration in the restoration [43, 192]. Similar to the core-veneering crowns, the stresses in the veneering porcelain still play a dominant role in the prosthetic longevity. In spite of certain differences between the test methodologies, all studies have shown that the

properties of the veneering porcelain influence the ultimate structural strength of the samples. To toughen the porcelain layer, Zhang et al. [102] and Wu et al. [115] proposed to optimise the topological configuration of FPD to enhance the fracture resistance, in which weak porcelain was replaced by strong zirconia. Their studies demonstrated much better fracture resistance of FPD structures made by the optimized material combination.

(b) Effect of geometrical designs

From a perspective of structural strength and longevity, the connector shape of partial dentures is a key concern as the highest stress is more likely to be concentrated in the connector area. Connector size and design have been recognized as the two main factors for optimizing the maximum load capacity (Figure 2.8 (c)). Miura et al. [60] found that the tensile stress values decreased in the designs with the expanded heights and widths of framework. On the other hand, Hafezeqoran et al. [194] observed that there was no significant difference with connector area. In addition to the connector size, Hafezeqoran et al. [194] also studied the effect of connector designs, and they found that a rounded height design had a higher load capacity than sharp embrasure. Pontic shape is another crucial design consideration to ensure the long-term survivability of the FPDs. There are three typical pontic designs, which are convex, biconvex and concave shapes. Inan et al. [195] suggested that the convex design had the best fracture resistance, followed by the biconvex and concave. In addition to the stress analysis, Thompson et al. [101] first utilized the XFEM technique to mimic the cracking path in the pontic.

Regarding retainer designs, Toman et al. [184] and Dal Piva et al. [187] compared the stress distribution between the single retainer and two-retainer configuration for FPDs (Figure 2.8 (d)), and the results indicated that the use of single retainer prevented stress

concentration on the interface between retainer and pontic. Inlay and onlay fixed partial dentures are two main replacement (retainer) configurations of FPDs, as shown in Figure 2.8 (e1) and (e2). According to the work by Field et al [23], both FPD designs exhibited similar stress in the bone region, however, the inlay design resulted in higher mechanical stress in the ceramic prosthesis. As shown in Figure 2.8 (f), the maximum fracture load of the inlay restoration was around half that of the onlay restoration [104]. In comparison with inlay preparations, onlay preparations, however, generally necessitate additional reduction of tooth tissues [63].

Regarding veneered FPDs, several laboratory and clinical studies have reported that increased fracture risk arises with the veneering porcelain due to the cohesive/adhesive failure. More veneer cracks indicated the higher risk of complete connector fracture. Some researchers examined the effect of design parameters on the fracture characteristics in the FPD components. For example, Messias et al. [64] compared the stress states between the straight and curved FPD framework, and they found that the curved geometry appears more prone to chipping or delamination of veneering material compared to the straight geometry. Also, similar to the veneered crown, veneer thickness ratio is critical for the fracture endurance of FPDs. Kalluri et al. [183] suggested that the framework thickness ratio of 1:1 resulted in a lower stress concentration and greater safety margin for failure..

(c) Effect of bonding interface

Wimmer et al. [188] and Assaf et al. [196] investigated the effect of cement on the stress levels in the three-unit fixed prostheses, and they suggested that the cement with a low stiffness in combination with a thickness as small as possible could increase the clinical

survival rate. The findings from Penteado et al. [189] also confirmed that the use of adhesive cement with a low elastic modulus could reduce the tensile stress concentration in the FPDs.

(d) Effect of loading conditions

Due to the complex loading conditions during biting and chewing, occlusal contact regions have been identified as one of the most important factors in the structural stability of FPDs. For example, Dittmer et al. [143] compared the stress states of FPDs with various contact points and locations. They found that the number and distribution of occlusal contacts significantly affected the stress distributions in the pontic and connector regions. Both fracture load and crack path are sensitive to the loading direction according to the literature [104]. Darwich et al. [185] and Velmurugan et al. [197] found that an oblique load generated higher stresses than vertical loads. In addition to the static occlusal loading, Zhang et al. [76] attempted to identify the dynamic load in the FPDs and the simulated load values showed good agreement with the clinical measurement data.

Similar to dental crowns, thermal-induced fabrication stress is a major factor leading to fracture of veneered FDPs. For example, Dittmer et al. [89] found that the thermal stress induced by the veneering process would influence the marginal and internal fit of the FDP. Koycu et al. [88] and Nabih et al. [198] investigated the stress distribution in the inlay-restored molar under thermomechanical loads. Borges et al. [100] studied the effects of different veneering techniques on the fatigue behaviours of the core-veneer all-ceramic FPDs, and they revealed that the conventional stratification technique was more prone to failure compared to the rapid layer and CAD-on techniques.

2.4 Orthopaedic applications

Orthopaedic implants, such as joint replacements and fixation devices, have become an excellent approach to replace injured or diseased bone and joints. The design of these implants requires consideration of the material's biocompatibility, chemical properties, mechanical properties as well as failure properties so that the implant is able to integrate with the native tissue and maintain their integrity during their lifespan. Among orthopaedic prosthesis, lower limb implants have a higher failure risk than others, e.g., spine and shoulder, as they carry greater physiological loading. Therefore, this section will focus on two main applications in the orthopaedic field for the load-bearing purpose, namely hip and knee arthroplasty. Table 2.6 summarizes the material properties of ceramic materials, e.g., Young's modulus, Poisson's ratio, tensile strength, etc., used in the hip and knee implants.

Table 2.6: Summary on material properties for ceramic materials used for total hip and total knee replacements.

	Density, ρ (kg/m^3)	Young's Modulus, E (MPa)	Poisson's Ratio ν	Tensile Stress σ_{TS} (MPa)	Fracture Toughness K_{IC} ($MPa \cdot m^{1/2}$)	Refs.
Alumina	3.850-4.635	350,000- 400,000	0.21-0.3	350-580	3.3-4.2	[74, 199- 204]
Zirconia	5.65-6.05	175,000- 250,000	0.23-0.3	450-700	2.9-16.0	[74, 200, 202, 205, 206]
ZTA	4.05-4.25	310,000-	0.22-0.24	600-1,248	4.1-6	[202,

		390,000				205, 207- 210]
ATZ	5.51	240,000- 261,000	0.27-0.28	775-1,163	8-12	[18, 202]
Y-TZP	6.00-6.05	210,000- 223,000	0.30-0.33	700-1,500	4.5-20.0	[202]
Si ₃ N ₄	3.0-3.4	270,000- 330,000	0.24	765	6	[38, 202]
HA	3.16	40,000-48,000	0.27-0.3	113-189	0.6-1.1	[200, 211, 212]

2.4.1 Hip implants

The continuously increasing necessity of hip and knee prostheses due to the worldwide rising aging population and increased accident rates have drawn considerable attention to improving the biological and mechanical performances of joint implants. Total hip arthroplasty (THA) is a surgical procedure in which the fractured or diseased hip is entirely replaced with an artificial hip implant prosthesis, as shown in Figure 2.9 (a).

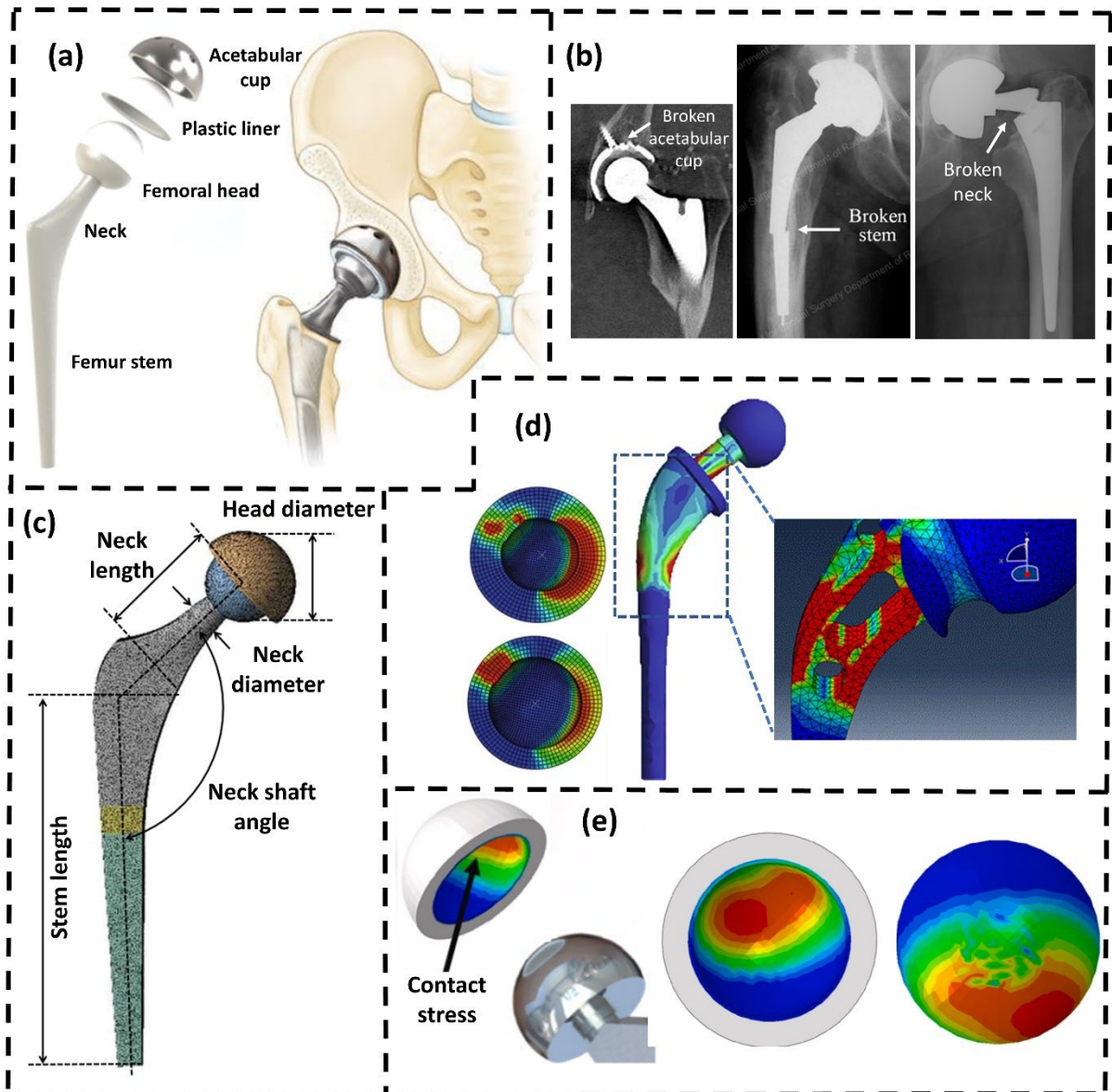


Figure 2.9: Finite element analysis used in the hip implant applications. (a) Schematic of a total hip replacement, indicating the different implant components. (b) Fracture sites of hip implants observed from X-ray image [213-215]. (b) Typical physiological loadings applied on the hip implant and femur bone (c) The common design parameters of a hip implant. (d) Representative stress distributions within the acetabular cup and femoral components [216,

217]. (e) Representative contact stress distribution at the interface between acetabular cup and ceramic head [218].

Due to the inherent brittleness of ceramic materials, several clinical studies reported that 10-12% of THA prostheses had experienced mechanical failure (as shown in Figure 2.9 (b)) [213-215]. Such outcomes have resulted in computational studies assessing and optimizing the strength of prostheses and will be reviewed in the following sections and tabulated in Table 2.7.

Table 2.7: Summary of numerical studies on fracture predictions/analyses of hip/knee implants made of bio-ceramics.

Research aims	Loading type	Contact condition	Failure criteria	Refs.
Design optimization	Static	Frictionless	MPS	[29, 219]
		0.3-0.35	MPS	[8, 27, 220]
		Bonded	MPS	[35, 39, 110]
	Cyclic	0.2-0.35	Stress based fatigue criterion	[33, 34]
	Impact	-	MPS	[78, 208]
Material selection	Static	0.3	MPS	[18, 38]
	Cyclic	-	von Mises stress	[38, 200, 204, 221]
Contact interface	Static	0-0.4	MPS	[10, 37]
	Cyclic	Element-dependent	Stress based fatigue criterion	[50, 203]
	Impact	0.05-0.4	MPS	[222, 223]
		Bonded	Stress based fatigue criterion	[75]
Loading scenarios	Static	0.04-0.27	MPS	[28, 49, 224]
		Bonded	MPS	[51]
	Cyclic	frictionless	Strain based fatigue	[29, 81]

		criterion	
Impact	Frictionless	MPS	[74, 201]
		von Mises stress	[82, 206, 225]
	0.04-0.06	MPS	[28, 49]

2.4.1.1 Effect of material selection

For load-bearing biomaterials, the transfer of force should take place in a physiological way [226]. In other words, the bone's integrity needs to be maintained, especially on the artificial interface between the implant and the bone. The majority of failure sites are found to be located on such interfaces because of the abrupt change in mechanical stiffness of the facing substrates. Therefore, the biomaterials used in orthopaedic implants need to be evaluated carefully. On the basis of tissue-implant reaction, the bioceramics can be generally classified as: (i) bioinert, and (ii) bioactive [227]. Bioinert ceramics, such as zirconia and alumina that do not encourage interfacial bonding amongst bone and implants, have been extensively used as implant materials for hip/knee prostheses owing to the bioinert nature, adequate mechanical stiffness, and excellent wear resistance. Regrettably, alumina (Al_2O_3) shows mediocre strength and fracture toughness which could potentially lead to catastrophic failures in orthopaedics. In line with this, many researchers have studied the effect of adding ceramic stabilizers to enhance the mechanical strength of pure Al_2O_3 . Vogel et al. [18] examined the stress and strain distribution in the implant with different bioinert oxide ceramics, e.g., Alumina, ATZ and ZTA. According to their results, both ATZ and ZTA exhibited a lower tensile stress magnitude than the alumina, which suggested a lower fracture risk under the daily functional loading. More recently, silicon nitride (Si_3N_4) showed excellent mechanical characteristics and non-toxic behaviours, which has become a potential candidate for load-bearing applications. Zhang et al. [38] studied the reliability of hip

resurfacing prostheses made by alumina and Si_3N_4 ceramics, and they found that Si_3N_4 had a lower fracture probability than alumina implants.

Bioactive ceramics are widely used as the coating material to promote the osseointegration and tissue growth, thereby minimising frictional sliding. Moreover, the coatings significantly help improve stress-strain distribution and fatigue strength, and reduce stress-shielding effects by a proper distribution of forces from implant to bone [228, 229]. Le Cann et al. [10] demonstrated that hydroxyapatite (HA) coating could reduce the macro-roughness of the implant to an appropriate level, thus avoiding excessive stress concentration. Darwich et al. [75] showed that the coating layer increased the safety factor of implant fatigue by 12.73%.

2.4.1.2 Effect of geometrical designs

Many researchers have made great efforts to optimise the geometrical designs of the implant to reduce fracture risks. Typical artificial THA consists of several common parts, namely acetabular cup, liners, femoral head, neck and stem, as shown in Figure 2.9 (a) and (c). According to the open literature, fracture sites can be usually found in both acetabular and femoral components (Figure 2.9 (b)). Han et al. [27] evaluated the implant stability according to the size of the acetabular component, and they found that increasing the size of the acetabular components could reduce the ceramic surface stress and lower the risk of impingement. Mathias and Tabeshfar [203] produced a novel acetabular cup with a ceramic-to-ceramic bearing to enhance the fatigue and wear resistance. The maximum tensile stress in the acetabular cup was reduced by 24% with a proper design (Figure 2.9 (d)). Moreover, neck-shaft inclination angle also affected the stress distribution in the acetabular cup and potentially initiate cracking in the cup [110]. Al-Wally et al. [225] found that a great

inclination angle may lead to fracture of the ceramic liner and head, and consequently, they determined the safe zone of the inclination angle to be less than 55 degrees.

In addition to acetabular cup design, femoral component is also critical to implant longevity. Several researchers simulated crack initiation and propagation in femoral neck and head regions using XFEM and phase-field method, and the simulated crack path exhibited good agreement with clinical X-ray images [29, 81]. Femoral neck length, stem length and shape are three parameters related to the fracture resistance of the overall implants. Various studies concluded that the combination of long neck length with a short stem design had better long-term reliability [34, 230]. Senalp et al. [33] compared four stem shapes with varying surface curvatures under both dynamic and static loading. The results showed that the optimum stem design could not only reduce the sliding of the implant between bone and cement, but also relieve the stress in the stem and further extend the fatigue life.

2.4.1.3 Effect of interface contact

Cement is used to bond the implant stem and the bone together and the degradation of cement strength affects the load transfer mechanism. Pal et al. [37] examined the effect of different implant-bone interfacial friction conditions; and found that the full implant-bone contact might lead to high tensile stress in the implant, which could further cause fracture, especially in the neck region. Hung et al. [50] investigated the effect of cement-implant bonding interface on fatigue failure. In their study, the progressively changed interface elements were introduced to the FE model to simulate the debonding of the cement-stem interface. The results revealed that the major crack site was in the proximal anterior-medial regions and at the distal prosthesis tip.

Apparent from the chemical adhesion of cement to the implant surface, geometrical adhesion is another factor that cannot be ignored [231]. Yamako et al. [232] developed a patient-specific model that explored the damage accumulation on the cement mantle based on the CT images. They concluded that the debonding course is the first step of damage accumulation, followed by the subsidence and micromotion of ceramic stem, which finally leads to the implant loosening and failure.

The contact between different components of implants is another factor which may influence the longevity of any prosthesis. High contact stress has been identified as one of the main reasons causing fracture of hip implants (see Figure 2.9 (e)). Contact stress is generated by the direct contact between hip head and cup rim during physiological movements [222]. Therefore, the failure risk of the ceramic components could be reduced by using a frictionless gap condition at the interface. This finding also emphasized the importance of lubrication between the contact implant components [35, 39, 110].

2.4.1.4 Effect of loading conditions

As discussed above, computational tools showed excellent capability of predicting mechanical failure and optimising implant geometries and material selections when a realistic load condition is known. These loads can vary notably between individual subjects and are highly dependent on the type and level of activities [8]. A number of researchers investigated the effects of different loading spectrums. For example, Katz et al. [51] predicted the mechanical responses of hip implants under hip contact loads with different angles. Todo and Fukuoka [35] studied the failure risk of the implant by considering bone adaption under static physiological loading. Dickinson et al. [49] explored the strength and reliability of a ceramic prosthesis under various loading scenarios, including static ramp loading with different

orientations, impaction loading and frictional torque loading. Based on the FEA results, they developed a physiologically representative mechanical test to simulate the ideal and worst-case loading and support *in vivo*.

Several studies showed that the implant predicted to be safe against failure under static loading may actually fail under dynamic repetitive loadings. For example, Elkins et al. [28, 223] and Brown et al. [78] studied the implant failure due to hard-on-hard impingements. They found that the stress magnitude increased linearly with increased cup tilt and cup anteversion. In some extreme cases, the peak stress values approached 1,000 MPa leading to the fracture of ceramics. In addition, they found that the cup orientations are most susceptible to liner fracture propagation for several impingements [28]. Uribe et al. [74, 209] carried out a series of studies to investigate the effect of dynamic loadings on the fracture of ceramic hip prostheses. The influence of cup-head mounted angle and material on implant damage induced by mechanical shocks was studied. The results revealed that the safe region of the mounted angle is between 45° and 60° under various loadings. Kalayarasan et al. [82] predicted the fatigue life of hip prosthetics subjected to various dynamic loading cycles, e.g., climbing stairs and knee bending. They found that alumina femoral heads exhibited high durability in all these loading scenarios.

2.4.2 knee implants

With the success of the hip prosthesis, similar material configurations have been extended to total knee arthroplasty (TKA), as shown in Figure 2.10 (a). According to clinical reports, the most prevalent complication encountered is implant loosening, which is directly

related to osteolysis. Numerous evidence indicates that wear particles generated by the articulating surfaces and metal allergy had adverse effects on osteoblast function and stimulate osteoclast recruitment. To address these issues, ceramic implant components exhibited promising results with increased wear resistance and long-term survival. However, it should be noted that ceramic bearings are less commonly used in TKA than THA due to higher implant failure risk caused by greater loadings in the distal region [227]. Facing the brittleness and relatively low fracture toughness of ceramics, the risk of fractures caused by stress peaks has to be assessed precisely. A number of researchers adopted computational tools to evaluate the stress peaks in the prosthesis and a representative FE model is shown in Figure 2.10 (b) [216, 217, 233]. They suggested that the highest stresses were mainly caused by intraoperative impaction loads. This section will review numerical studies on the fracture of knee implants.

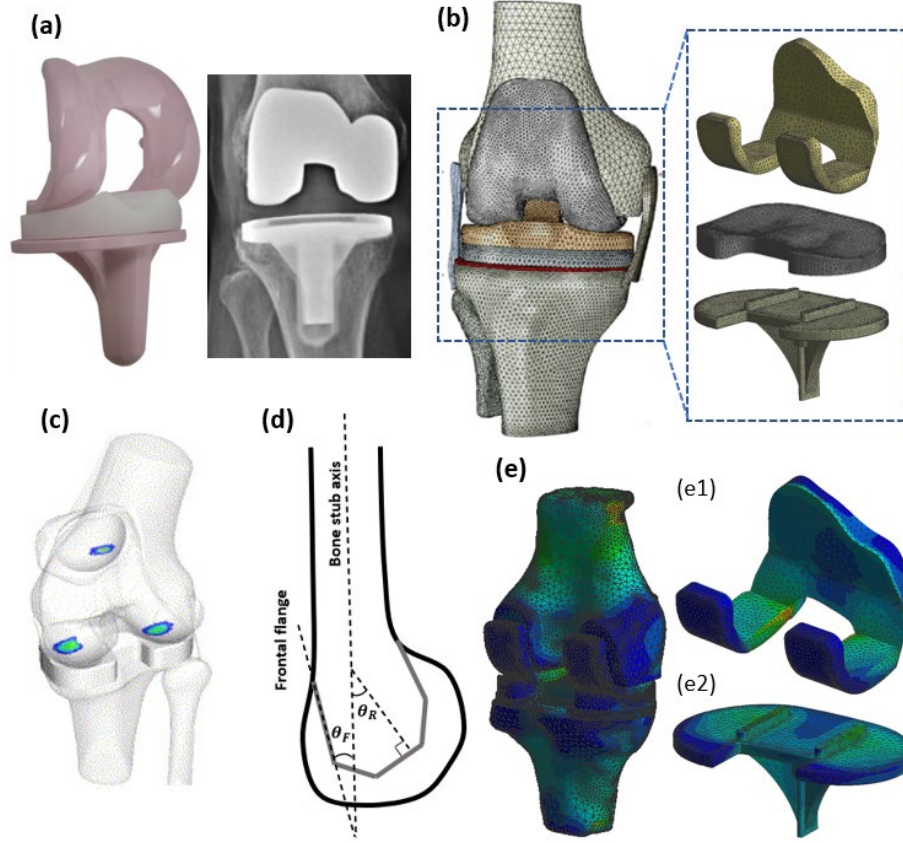


Figure 2.10: Finite element analysis used in the knee implant applications. (a) A representative ceramic knee implant [234]. (b) Schematic of a total knee replacement, indicating the different components [233]. (c) The contact pressure between different components. (d) The resection angle, θ_R , and flexion angle, θ_F , of the prosthesis. (e) The stress distribution in the knee implants. (e1) Femoral component, (e2) Tibia component.

As shown in Figure 2.10(c), higher stress regions occur in the area of force transmission and in the median plane. Stress peaks can be minimized through proper material composition, adequate implant design and optimum force transmission between bone and implant. Kumar and Sarkar [205] compared the compressive strength of various ceramic implant materials

and they found that zirconia-toughened alumina had better performance compared to pure alumina, zirconia and Si₃N₄.

Intraoperative impaction of ceramic components during placement using an impactor (hammer) creates a considerable challenge to the ceramic implants. From a geometrical design point of view, to increase the implant safety, the femoral resection angles (shown in Figure 2.10 (d)) should be prepared very precisely, in particular anterior saw blade deflection has to be avoided. Unintentional deflection of saw blades could lead to higher resection angle of distal femur than desired, which causes bending of the femoral component during implantation. Klues et al [208] carried out FE analysis to simulate placement of the femoral component to evaluate the influence of distal femur preparation on maximum principal stress which is closely related to the tensile fracture of implant. In addition to the resection angle, cross sectional contact area is another important factor. Nabrdalik and Sobocinski [235] suggested that the value of stress in the implant with 27 mm cross section radius is remarkably lower (10-12%) than in case of 17 mm cross section radius, which resulted in the increased durability of endoprosthesis.

Intraoperative impaction is a highly dynamic process, the reduction of velocity and weight of hammer is recommended to minimize the influence of impaction related stress concentration. In addition, by using a 5 mm thick silicone cover between impactor and the femoral component, a remarkable decrease of vibration can be observed which lead to a 54%-68% reduction in peak stress [201]. In addition to the impaction pulse, the postoperative in-vivo loads play a vital role on the long-term stability of knee implants. Figure 2.10 (e) shows the stress distribution in the ceramic components in the knee implants. Klues et al. [236] compared the stress concentrations of implant under different worst case scenarios including

malposition, bone defects and stumbling. The simulation results revealed that the principal stress caused by stumbling was 12.6 times larger than the normal gait. Cement layer is critical to the load transfer between the components of knee implants. Schultze et al. [237] conducted 2D and 3D FE analysis of artificial knee joint with different cement layers, and they suggested that a thicker cement layer could reduce the stress in the ceramic femoral component.

2.5 Bone tissue engineering applications

Bone is a hard tissue that provides structural integrity to the body and sustains physiological loadings. Segmental bone loss caused by trauma, infection or tumour, commonly leads to significant disability in patients. In the case of long bone injuries, a significant bone loss can be found because the natural healing/remodelling potential of bone cannot be accomplished by itself. To reconstruct the defects, autografts and allografts are conventional options available for bone repair. Nevertheless, the corresponding problems, e.g., pain and immune rejection, have encouraged the development of artificial bone-like substitutes such as bioceramic scaffolds. They have demonstrated the potential to provide a suitable environment during bone healing and subsequent remodelling. Table 2.8 summarises the material properties of ceramic materials used in bone tissue scaffolds. It can be seen that Young's moduli of bulk bio-ceramics are substantially higher than that of human bone, thereby potentiating inadequate load transfer and stress shielding in bone. To avoid this, it is important to fabricate porous ceramic structures with lower effective elastic properties than the equivalent bulk material. In line with it, Genet et al. [238] proposed a Sanchez-Palencia theory based homogenisation approach for estimating effective stiffness and mechanical

strength of porous ceramic structures, thereby establishing a reliable tool for optimising mechanical properties of the whole structure.

Table 2.8: Summary on material properties for bio-ceramic materials currently used for bone tissue scaffolds.

	Density, ρ (kg/m^3)	Young's Modulus, E (MPa)	Poisson's Ratio ν	Tensile Stress σ_{TS} (MPa)	Fracture Toughness K_{IC} ($MPa \cdot m^{1/2}$)	Refs.
Zirconia, 3Y-TZP	6,000	200,000	0.28-0.3	1,000-1,400	6.0-15	[2, 73]
Sintered HA	3160	14,690 - 86,000	0.28	56-120	0.8-1.2	[15, 44, 238, 239]
Polymer infiltrated HA	-	296.1-3,690	0.3-0.35	-	-	[70, 240]
β -TCP	3070-3140	24,600-84,000	0.28-0.3	18-46	0.79-1.46	[16, 30, 239, 241, 242]
Polymer infiltrated β -TCP	-	250-6,360	0.3	-	-	[30, 241]
Calcium phosphate, CaP	3140	455	0.33	12-16	0.39-0.73	[26, 62]
Sr-HT-Gahnite	-	33,000-47,000	0.26-0.3	97	1.24	[107, 243]
Silicate-based bioactive glass (13-93)	-	(13,000)62,000-70,000	0.25-0.28	40	0.6	[17, 25, 244]

From a design perspective, bone ingrowth and mechanical strength are the two most essential criteria for orthopaedic scaffolds. From in-vivo studies, early stress stimulation can play a crucial role in long-term bone healing response [245]. However, excessive stress could lead to catastrophic fracture of ceramic scaffold. Substantial efforts have been devoted to regulating the mechanical stress in the bone scaffold to obtain optimum bone growth outcome while also preventing failure and fracture. This can be achieved by selecting the optimal base materials and appropriate structural designs that align with individual anatomy and physiological loadings. This section will discuss recent progress in computational investigations focused on mechanical strength and fracture failure of bone tissue scaffold, as summarised in Table 2.9.

Table 2.9: Summary of numerical studies on fracture analyses and predictions of ceramic based bone scaffolds.

	Research aims	Loading conditions	Failure criteria	Refs.
Material effects	Various ceramics	Uniaxial compression	MPS	[26, 44, 62, 107]
	Polymer infiltration	Uniaxial compression	MPS von Mises stress	[16, 240] [61, 70]
Structural optimization	Cellular design	Uniaxial compression	MPS	[45, 73, 238]
	Strand diameter and spacing	Uniaxial compression	MPS	[72]
	Porosity and Pore size	Uniaxial compression	MPS	[17, 71, 243] [246]
			GTN	[2, 77, 247] [248]
		4-point bending	MPS	[25]

		In-situ	MPS	[249]
Fabrication process optimization	-	In-situ	MPS	[107, 108]
Other	Fracture prediction	Uniaxial compression	MPS	[15, 26, 30] [107, 239] [250]
			Fracture energy	[118]
		3/4-point bending	Failure strain	[238]

2.5.1 Material selection

(a) Various ceramics

Ceramic scaffolds have been developed over many years for bone tissue engineering [16, 251, 252]. Some properties, such as bio-inertness, biocompatibility and hydrophilicity make them suitable for fabricating tissue scaffolds [73]. Yttria-doped zirconium dioxide (YSZ) ceramic, particularly in the form of 3Y-TZP, is amongst the most interesting candidates for its excellent mechanical and physical properties [2]. Bio-active ceramics, e.g., Hydroxyapatite (HA) and Tricalcium Phosphate (TCP), have gained growing attention in recent years owing to their superior osteoconductive properties and ability to support bone growth. However, bio-active ceramics are often of a relatively low mechanical strength compared to dense ceramics, e.g., zirconia. Miranda et al. [15] analysed the fracture modes under uniaxial compression of a HA scaffold. They found that Mode-I failure caused by tensile stress is a primary failure type of such scaffolds. Based on this study, Miranda and the coworkers [239] utilized FEM to compare the fracture behaviours of robocats scaffolds made of HA and β -TCP under different loading scenarios, e.g., compression, tension, and shear.

According to their results, both of tensile and shear stresses could lead to premature failure of the scaffold. More recently, Strontium-hardystonite-Gahnite (namely Sr-HT-Gahnite) has been developed to fabricate bone tissue scaffolds. Sr-HT-Gahnite is a highly porous and biocompatible bio-ceramic that has similar mechanical properties to bone tissues. To evaluate its mechanical strength, Entezari et al. [243, 253] proposed a series of numerical studies and they suggested that Sr-HT-Gahnite had a similar mechanical strength to that of cortical bone, highlighting the promising potential of Sr-HT-Gahnite in bone tissue engineering.

(b) Polymer infiltrated ceramics:

To increase the toughness of pure HA and TCP, infiltrating the brittle scaffold structures with a biocompatible polymer offers an attractive option. Polycaprolactone (PCL) and Polylactic-acid (PLA) have been considered as the most commonly used infiltration material to improve the mechanical behaviours [30, 241]. For example, Martinez-Vazquez et al. [16] and Eshraghi [70] found that threefold and sixfold increases in scaffold compressive strength following PCL and PLA infiltration, respectively. Martinez-Vazquez et al. [16] and Lowe et al. [61] reported that the infiltrating polymers into the porous TCP structures could enhance the strength of the composite materials (151 MPa) to make it close to that of cortical bone

2.5.2 Structural design

The scaffold architectures, such as cellular configurations and porosity/pore size, are critically important to providing sufficient mechanical stiffness and strength, as well as biotransport properties for vascularisation and tissue remodelling. To fulfil these requirements, an interconnected structure is essential for the scaffold to allow the transport of nutrients and waste while assuring tissue ingrowth. The design of appropriate cellular

configuration, pore size and porosity play a key role in balancing the overall stiffness/strength and permeability [108, 243, 254].

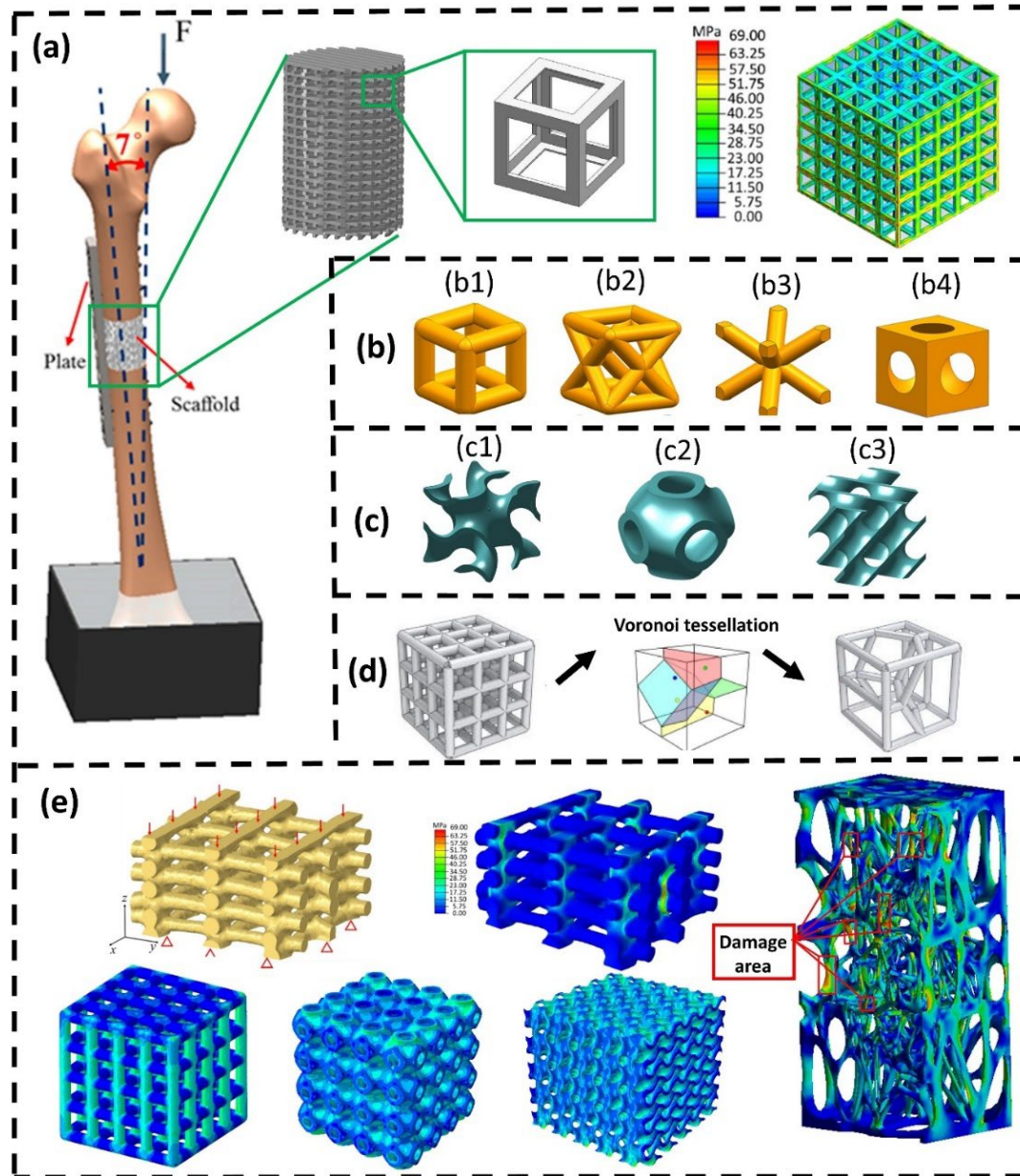


Figure 2.11: (a) Typical femoral model with segmental defect implanted using a tissue scaffold. (b) Cubic unit cell topologies; (b1) Cubic close packed (CCP), (b2) Face-centred cubic (FCC), (b3) Body-centred cubic (BCC) and (b4) spherical hollow cubic (SHC) [255]. (c) Triply Periodic Minimal Surface (TPMS) unit cell topologies; (c1) Gyroid, (c2) Primitive,

(c3) Diamond [256]. (d) Development of Voronoi unit cell from regular lattice structural with Voronoi tessellation [257]. (e) Representative FE results for the tissue scaffold [116, 258, 259].

(a) Scaffold cellular configuration:

The unit cell is a basis of porous structures, which can be divided into non-parametric design and parametric design, as shown in Figure 2.11 (b-d). Non-parametric designs, such as diamond/face-centered-cubic (FCC), body-centered cubic (BCC), and octahedron (OC), etc., have been widely studied in the literature, as shown in Figure 2.11 (b). Ensuring structural integrity under the physiological loadings is the primary requirement for the load-bearing scaffold in bone tissue engineering. A number of researchers have studied the fracture behaviours of non-parametric scaffolds by using various computational tools (as shown in Figure 2.11 (e)). For example, Montufar et al. [45] investigated the fracture mode under compression of regular and shifted orthogonal scaffolds. The authors stated that shifted scaffolds performed similarly to regular ones in the transverse direction but were less mechanically reliable under the longitudinal direction. It was found that the fracture site of scaffolds first occurred in the struts that carry the tensile load, and the maximum tensile stresses are located on the top and bottom surfaces of the horizontal rods [250]. Fabris et al. [73] evaluated the mechanical performance of periodic open cellular scaffolds and optimized their geometries to fit different clinical scenarios. Uth et al. [72] performed an optimisation study to identify the optimum combination of strand diameter and spacing.

Biological and mechanical functions are often two conflicting requirements of bone tissue scaffolds, which necessitates an optimal trade-off between these two properties in load-bearing applications [2, 248]. Recently, Entezari et al. [249] introduced a modular design

strategy to fabricate a load-bearing scaffold that supports the hydrogel and ceramic based hybrid structure to withstand the various *in-vivo* loading while maintaining a proper biological environment.

Compared to non-parametric design, parametric design refers to cellular structures that can be generated with specific functions and algorithms, which possess a more complex architecture. The advances in additive manufacturing make it possible to fabricate such intricate structures. There are two main methods to design the parametric porous structure in terms of different functions and algorithms. Triply Periodic Minimal Surface (TPMS) and Voronoi-Tessellation are two typical examples that exhibit some advantages, such as high randomisation, functional internal connectivity, and excellent mechanical properties, as shown in Figure 2.11 (c) and (e).

Structures with TPMS consist of periodic unit cells with a minimum possible surface area and have smooth surfaces, which are excellent structures for cell proliferation (shown in Figure 2.11 (e)) [260]. The FEA results showed that the mechanical properties of TPMS scaffolds were close to bone [261]. Further, Cai et al. compared the mechanical properties and bone ingrowth performance of four kinds of TPMS structures (Gyroid, Primitive, Diamond and I-wrapped package(I-WP)); and their results revealed that the Gyroid surface TPMS had the most flexible design space leading to a better mechanical strength compared to the Primitive, Diamond and I-WP counterparts. According to FEA, TPMS structures (P- and D-surface) exhibited different effective Young's moduli under stretching and bending, shown as Figure 2.11 (e) [262]. The failure mechanism of the stretching structure represented by the P surface was explored; and the results showed that the P surfaces were destroyed in a layer-by-layer mode under ultimate loading pressure [263, 264].

In terms of Voronoi design, it appears to be one of the most comparable designs to bony structures in the literature. Utilising Computer-Aided-Design (CAD) codes, a 3D porous interconnected scaffold can be created based on the Voronoi algorithms (Figure 2.11 (d)). Such Voronoi scaffolds appear to better match the main histomorphometric indices of bone, especially trabecular bone, such as bone volume ratio, bone surface-to-volume ratio, etc. [265]. The mechanical properties, such as Young's modulus and compressive strength, of the Voronoi scaffolds were evaluated by Gomez et al. [71]. Maliaris et al. [266] carried out the compression tests of the Voronoi scaffolds and found the critical load of Voronoi based porous structures increased by nearly 300%.

(b) Porosity and pore size:

In addition to the unit cell topologies, porosity and pore size are also important structural factors affecting the biomechanical properties of scaffolds (Figure 2.12 (a)). Firstly, the stiffness of scaffold is closely related to the porosity and pore size [244, 267]. Cui et al. [246] and Li et al. [268] showed that increase in either porosity or pore size can lead to degradation in global stiffness and fracture strength of scaffold, and they noted that the changes in porosity had a more pronounced impact. As shown in Figure 2.12 (b), the fracture strength of such scaffolds can be enhanced by optimizing porosity and pore [242, 269]. Deliormanli [17] performed a stress analysis for the robocasting fabricated scaffold with varying pore widths and layer spacing parameters, which can be used to optimise geometrical parameters and determine the most suitable ones for the replacement of natural tissues.

Not only does the porosity affect the mechanical properties, but also the bone formation performance. Entezari et al. [243] suggested that both compressive strength and permeability can be enhanced via selecting the appropriate porosity and pore size. They determined the

optimal combination which can improve the mechanical strength by 70% without sacrificing nutrition permeability. Domez et al. [71] and Liu et al. [247] optimised the porosities of Voronoi scaffolds to achieve an optimum mechanical strength and mass transport abilities.

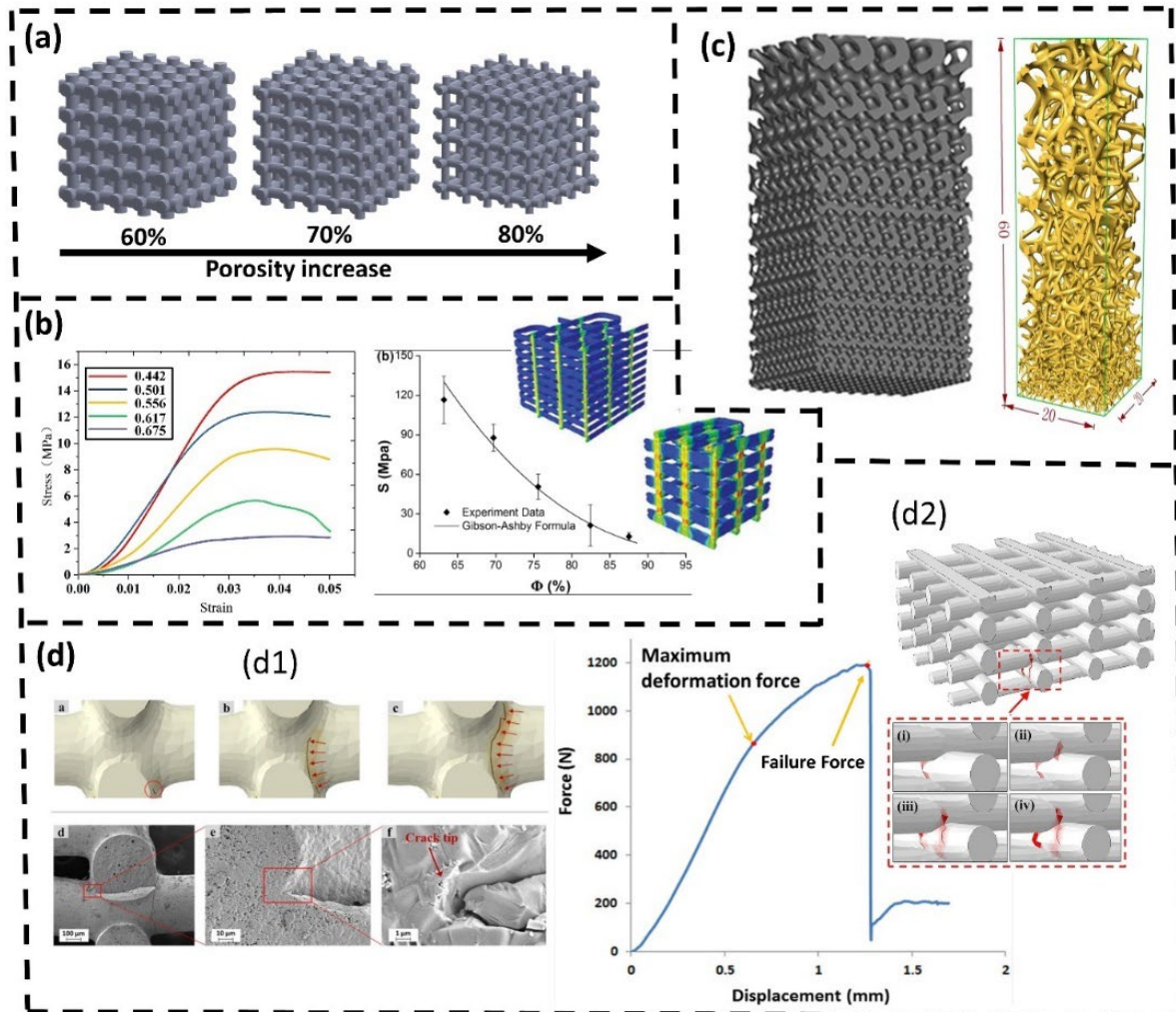


Figure 2.12: (a) Scaffolds with different porosities, 60%, 70% and 80%, respectively; (b) Relationship between scaffold strength and porosity [258, 265]. (c) Designed scaffold with gradient porosity; (c1) TPMS scaffold [270]. (c2) Voronoi scaffold [265] (d) Comparison of crack pattern for designed and printed (according to CT scan) models [107]. (d1) The crack

patterns from simulation and SEM observation; (d2) Force-displacement curve of scaffold and the simulated crack path obtained by XFEM.

At present, the design of porous scaffold has attempted to mimic the natural bony tissue biomechanically, which often has a non-uniform porous structure, the density of which gradually increases from the inner cancellous bone to the outer cortical bone [71]. Thus, a number of researchers developed gradient scaffold and utilized FEA to evaluate the mechanical properties compared the uniform scaffolds, as shown in Figure 2.12 (c). For example, Xiao et al. [25] compared the mechanical strength of scaffolds with uniform and gradient porosities and showed that the gradient scaffold had greater flexural strength. Similar results were found by other researchers and suggest that the mechanical properties of gradient scaffolds are suitable for bone implants [246, 264, 266].

2.5.3 Fabrication process

The production of ceramic scaffolds can be made through subtractive or additive manufacturing technologies. Note that these direct processes allow for obtaining the green body, meaning that a subsequent sintering step is needed to sinter/consolidate the ceramic materials. Additive manufacturing (AM) technologies exhibit unique advantages in producing customised scaffolds for each patient with desired architectures. However, the uncertainties during the fabrication process could lead to pre-cracks and undesired geometrical variance in fabricated scaffolds. Regarding the former factor, Petit et al. [26] characterised the effects of pre-existing defects on the fracture behaviours of ceramic scaffolds subject to compression tests. The results revealed that the main crack in the brittle-like materials would propagate parallel to the compression direction. In addition, imaging techniques, e.g., X-Ray Micro Tomography (XMT) showed the potential ability to characterize the complex crack paths in

ceramic laminated structures which could provide some basis for the FE modelling [118]. In terms of the geometrical variance, micro-CT is a powerful tool to examine the change in the geometry during the fabrication process and the scan images can be used to reconstruct the 3D model for further FE analysis. For instance, Entezari et al. [107, 108] utilised XFEM to quantify the fracture strength of scaffolds and took into account the geometric variations induced by the fabrication process with the help of u-CT, as shown in Figure 2.12 (d).

2.6 Current challenges and outlook

It has been noted that enormous research effort has been devoted to the studies on fracture prediction of the ceramic bio-structures in literature. Most of these studies adopted FEA to investigate the stress states of the bio-structures under the physiological loadings, as the stress is one of the most critical indicators for examining the safety of such structures. In addition to the conventional linear FE analysis, more advanced computational modelling approaches, based on linear elastic fracture mechanics, have been developed to mimic the crack formation and subsequent propagation. It has been shown that numerical modelling methods are gaining growing popularity over recent years. Nevertheless, there are still some key challenges remaining to be tackled, as follows:

Comprehensive understanding on how ceramic materials could fail signifies a major research topic for better designing ceramic structures. The micro-structures inside ceramic materials, such as aggregates, voids, microcracks, etc., play a significant role in determining the onset of crack nucleation and propagation [271]. High-resolution microscopic analysis techniques, such as micro-CT, SEM, TEM, etc., enable to capture the micro/nano-structures

of bio-ceramics. According to the images from such techniques, a more accurate imaged-based FE model can be created and would have great potential to more precisely simulate the cracking process at a relatively small length scale.

In addition, combining the fine scale models (nano or nano-scale) with macroscopic behaviour can be important to mimic fracture process more realistically. Hence, one future direction of research is the establishment of fracture models across different length scales. The main challenges of futuristic multiscale methods can be to develop effective techniques to transfer through different length scales when damage occurs, which needs to choose suitable discretisation. Another challenge would be to overcome the high computational cost, especially when involving multiscale optimisation.

Although various 3D printing techniques offer exceptional advantages and great potential for fabricating highly sophisticated architectures, the printing quality still remains some concerns, especially for bioactive ceramics, such as HA. Some experimental studies suggested that the printed ceramics exhibited anisotropic mechanical properties due to the layer-by-layer forming process. In addition, some flaws/cracks can be observed, which may be caused by the thermal stress during the sintering process. A high-fidelity FE model may need to be developed for simulating thermal loading and get a more inclusive understanding of the anisotropic behaviour and crack formation caused by thermal loading during the fabrication and post-processing process.

Other key challenges of future fracture analysis techniques can be to develop more reliable and efficient methods to model the inherent stochastic properties of ceramics. Most of the computational techniques available for fracture in ceramic structures as discussed

above are based on deterministic methods. There have been relatively fewer efforts on statistical algorithms for fracture modelling.

Machine learning techniques, such as artificial neural network (ANN), have been effectively used for complex problems in engineering and material sciences. These stochastic approaches are based on computational intelligence and machine learning tools by correlating the system input parameters to the outputs by means of mathematics and statistics methods. Machine learning-based approach shows promising applications in predicting fracture behaviours of bio-ceramics owing to its excellent reliability, accuracy, and robustness.

Chapter 3: Modelling of stress distribution and fracture in dental occlusal fissures

This study is aimed to investigate the fracture behavior of natural mineralized tissue, enamel, under simulated occlusal load in relation to various interacting factors including fissure morphology, cuspal angle and the underlying material properties of enamel. XFEM method was adopted to analyze the fracture load and crack length in dental models with different cusp angles, fissural morphologies, and enamel material properties. The analysis results showed that fissures with larger curved morphology such as U shape and IK shape, exhibit higher resistance to fracture under simulated occlusal load irrespective of cusp angle and enamel properties. Increased cusp angle (i.e. lower cusp steepness), also significantly enhanced the fracture resistance of fissural enamel, specifically for the IK and Inverted-Y shape fissures. Overall, the outcomes of this study explain how the interplay of compositional and structural features of enamel in the fissural area contribute to the resistance of the human tooth against masticatory forces. These findings may provide significant indicators for clinicians and technicians in designing/fabricating restorative dental crowns and correcting the cuspal inclinations and contacts during clinical occlusal adjustment.

3.1 Introduction

Dental enamel, as the most highly mineralized tissue in the human body, mainly consists of hydroxyapatite nanofibers and traces of water and organic molecules. The crystalline structure as well as the high hardness and stiffness of enamel, endow it the capacity to

tolerate a range of lifelong mechanical, thermal and chemical stimuli while still maintaining its cutting and masticatory functions. However, due to its highly mineralized composition, enamel is a relatively brittle biomaterial with an elastic modulus in the level of 100 GPa and a toughness value comparable to that of glass [272]. The brittle nature and high susceptibility to mechanical failure presents a more critical problem in deep fissures located in the occlusal surface of molar and premolar teeth. In these fissural regions, the thickness of enamel is significantly lower than enamel cusp tips and proximal surfaces. Moreover, the sharp corners and narrow curvatures within the fissure system potentially create vulnerable sites of stress concentration and crack initiation in enamel.

The cusps of posterior teeth, bear substantial bending and flexural loads during functional and specifically eccentric parafunctional occlusal movements. These applied loads can theoretically generate a horizontal force component which can open up the fissural space and create tensile stress concentration and subsequent cracks at the base of the fissure. Although it is common to see cracking of the cusps to initiate from the fissural area in carious teeth, the prevalence of fracture in the fissural area of sound teeth is surprisingly low [273]. The resistance of fissural enamel with presumably weak structural design and brittle nature, against millions of chewing cycle loads of up to 1200 N is a thought-provoking phenomenon.

While occlusal enamel fissures seem to be susceptible sites for bacterial plaque retention, caries formation and crack initiation, their introduction into the dentition of heterodonts was a significant step in evolution which led to the transformation of canine-like teeth morphology of zyphodonts to the multicuspid dentition of heterodonts, with a broad diversity of tooth types and shapes [274]. This transformation enhanced the efficacy of the masticatory system

of omnivores and optimized the utilization of food caloric energy for an increased level of intricate physical and intellectual activities [275].

The genesis of occlusal fissures happens during the bell stage of the tooth formation process, through folding invagination of the inner enamel epithelium and the subsequent fusion and mineralization of adjacent developmental dental lobes [276]. While these fissures can display a range of depths and widths, from shallow grooves and fossae to deep and narrow pits and fissures, their morphology follows five main patterns [277], namely I-shape, U-shape, inverted Y-shape (IY) , IK-shape and V-shape.

Previous studies have revealed that enamel thickness and cusp size are the critical morphological factors involved in the fracture behavior of enamel [278]. Other studies have focused on the microstructural features of enamel including its hierarchical organization, the presence of micron-sized defects and the role of organic remnants, in the mechanical resistance and fracture behavior of enamel [278, 279]. However little is known about the effect of fissure geometry as well as the composition and material properties of enamel specially around the fissural area, on the resistance of the tooth against fracture. Therefore, the current study aims to investigate the fracture behavior of fissural dental enamel under simulated occlusal load in relation to various factors, including fissure morphology, cuspal angle and the underlying material properties of enamel.

3.2 Materials and Methods

3.2.1 Mineral density characterization and quantification

Extracted human premolar teeth were collected from oral surgery and orthodontics departments at Sydney Dental Hospital, The University of Sydney. The specimen collection

and experimental methods were performed in accordance with the ethics approval guidelines from Sydney local health district ethics review committee, protocol No X12–0065 & HREC/12/RPAH/106. Regarding specimen collection, each patient was provided an information sheets and informed consent was obtained from all subjects. Mineral density distributions of teeth were characterized using a high-resolution desktop microscopic computed tomography system (Skyscan 1172, Skyscan N.V, Aartselaar, Belgium) at an accelerating source voltage of 100 keV, a source current of 100 μ A, and an exposure time of 885 ms. Three hydroxyapatite discs with low, medium and high mineral densities were used for grey level calibration to determine the mineral density values of different parts of the tooth. Details of the employed phantoms are provided elsewhere [280].

Low energy X-rays were eliminated using an inbuilt filter equal to 1.0 mm thickness of aluminium and 0.05 mm of copper to restrict the spectral bandwidth of the polychromatic radiation. The equivalent monochromatic energy spectrum of filtered X-rays had an effective mean energy of 60 keV. The long axes of the teeth were placed parallel with the centre of rotation of the mounting device. During the scanning process, the samples were rotated over 360° at angular increments of 0.14°, generating 2570 two-dimensional shadow projections with an image matrix of 2000 pixels $\times$ 1048 pixels. These images were saved as 16-bit Tagged Image File Format (TIFF) and consequently exported to a 3D cone beam reconstruction program (NRecon software, version 1.4.4; SkyScan) for the tomographic reconstruction of the tooth and production of tomographic images. The tomographic reconstruction produced a dataset of slice views in 16-bit TIFF format, which were perpendicular to the specimen rotation axis and had a voxel size resolution of 8–10 μ m. Vertical bucco-lingual slice views were produced by re-slicing the reconstructed volume of

the whole image stack in FIJI (W.S. Rasband, U.S. National Institutes of Health, Bethesda, Md, USA, <http://imagej.nih.gov/ij/>, 1997–2011).

The produced tomographic images were consequently imported into MATLAB (MatLab R2012b 8.0.0.783, Mathworks, Natick, MA, USA) for the denoizing process which increases the signal to noise ratio of the micro-CT images. Denoising was performed using a method based upon total variation regularization [281, 282], with the following parameters: (regularization parameter) = 0/04. (initial penalty parameter) = 3.

The calibration of mineral density was implemented by measuring and averaging grey level values of selected images of each hydroxyapatite phantom, followed by plotting the obtained grey level values against the mineral density value of that phantom. Based upon the plotted values, a calibration equation was used to transform the grey level values of the images into true mineral density values [280].

Mineral mapping and color-coding of the tooth was performed using the colormap editor command in MATLAB by choosing Jet color map with fixed RGB (Red, Green, Blue) index values for all of the colorized images. The color codes were based upon the greyscale values and corresponding mineral densities of the specimen, thereby yielding a calibrated mineral map.

3.2.2 Finite element models

A bucco-lingual cross-sectional image was selected from the micro-CT dataset of an upper premolar tooth to construct the two-dimensional (2D) finite element (FE) models [283]. The anatomies of bone, enamel and dentine, were specified in the image processing software ScanIP (Simpleware Pty. Ltd, UK). Once surface refinement of masks for each component of

the model was completed, the FE model was exported as an IGES file for further modification in SolidWorks (SolidWorks Corp., USA). The periodontal ligament (PDL) was then created by offsetting the outline of the root section of the tooth [284, 285]. Five different geometries for the occlusal fissure including U shape, V shape, IK shape, I shape and Inverted Y (IY) shape, were modeled as shown in Figure 3.1(c). For each fissure geometry, nine FE models with varying cusp angles from 50° to 70° in an interval of 2.5° were constructed in SolidWorks. Nominated models of a tooth with the U shaped occlusal fissure and cusp angles of 50° and 70° are shown in Figure 3.1(a) and (b), respectively.

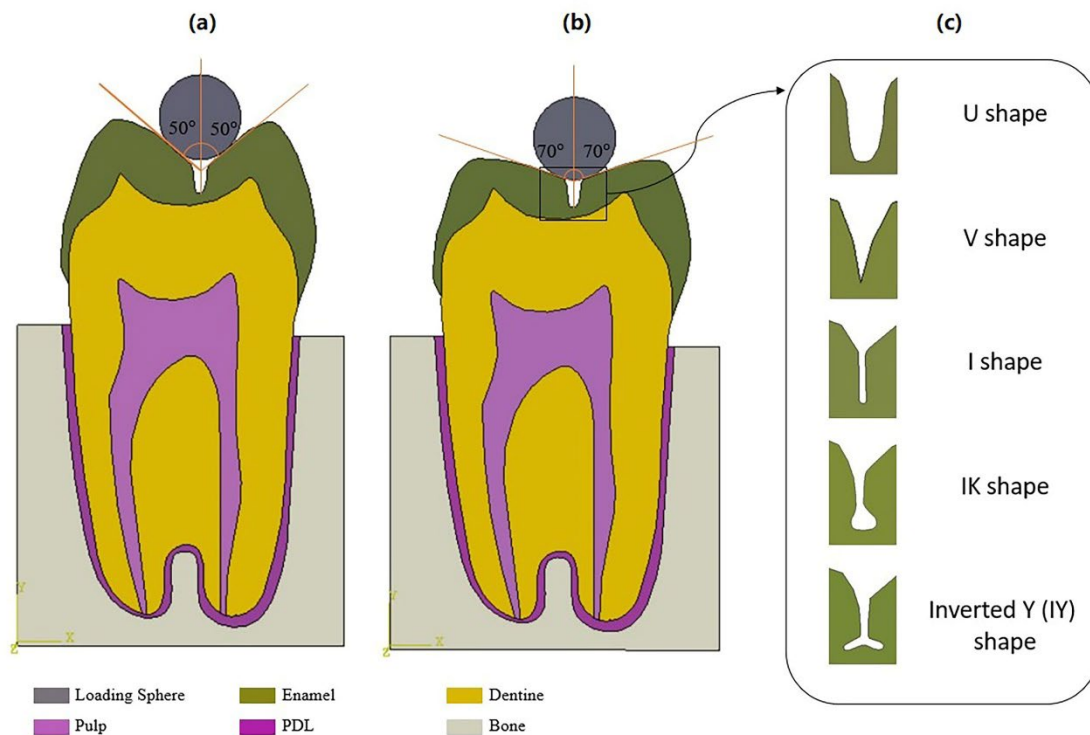


Figure 3.1: Finite element models of a premolar tooth with the U-shape occlusal fissure: (a) cusp angle 50° ; (b) cusp angle 70° ; (c) Five geometry types of occlusal fissure. The colors in the figure represent the bone, loading sphere and different parts of the tooth.

The FE models were meshed by using four-node bilinear quadrilateral elements. The mesh convergence test was conducted to determine the appropriate mesh size for tooth models by balancing the accuracy of results and computational cost [170, 285]. According to the results of the convergence test, the global mesh size was 0.09 mm for the tooth model and 0.2 mm for the loading sphere. Due to the complex geometry of fissure areas, the meshing refinement was further performed using a local mesh size of 0.03 mm. Consequently, the number of elements was 42,282 (Degree of freedom - DOF: 84,736) for the tooth model, and 440 (DOF: 934) for the loading sphere.

The models were loaded using a 5 mm diameter steel ball controlled by a downward displacement of 0.2 mm. As this finite element analysis was carried out to simulate the indentation process, the sphere model played the role of indenter ball. Therefore, the sphere model was set to be a rigid body and the contact between sphere (indenter ball) and tooth surface was assigned a friction coefficient of 0.3 in tangential direction [105]. All the FE models were kinematically constrained on the outer and bottom surfaces of the bone region [286, 287].

3.2.3 Material properties of the components of the FE model

The loading sphere was treated as steel, which was modelled to be linear elastic, isotropic and homogeneous [103]. Regarding the tooth model, all the materials were considered to be isotropic and homogeneous [105]. However, for the enamel, three regions of inner, middle and outer enamel were considered separately in order to reflect the non-isotropic nature as well as the gradient of the mineral density [276] and material properties which exist in natural enamel. These areas were determined based upon the mineral maps generated from microCT images of the tooth. Figure 3.2 shows the nominated colorized

mineral map of a buccolingual section of a premolar tooth. The mineral map (contour) displays the gradient of mineral density decreasing from enamel surface towards the dentin-enamel junction.

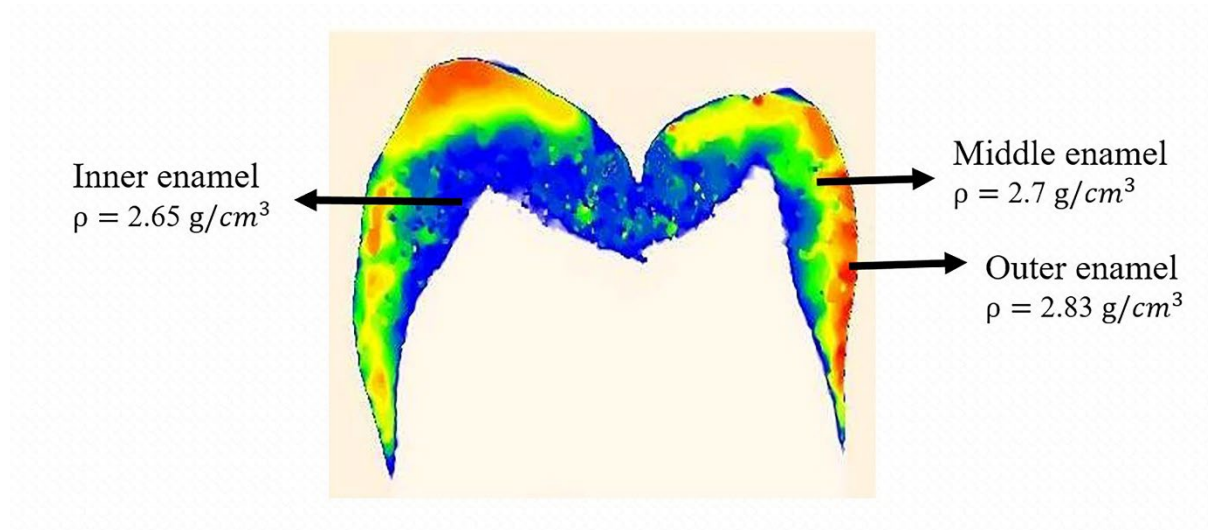


Figure 3.2: Colorized mineral map (contour) of a buccolingual section of a premolar tooth, generated from a microCT image. The mineral map (contour) displays the gradient of mineral density decreasing from enamel surface towards the dentin-enamel junction.

Table 3.1 shows the values for the mineral density and corresponding Young's modulus, fracture toughness and strain energy release rate in different areas of enamel. Previous studies have revealed the correlation between mineral density and Young's modulus in enamel [274, 276, 288]. Accordingly, the mineral density of enamel lies mainly within the linear portion of the mineral density versus elastic modulus curve [289]; and therefore, elastic modulus values can be calculated from the values of calibrated mineral density. The studies have also shown that the fracture toughness of enamel is correlated with the distribution of mineral density [290].

However, in contrast to the trend of Young's modulus, the higher density values translate to lower fracture toughness values [290, 291].

Table 3.1: Material properties of the components of the FE model are adopted from the literature [274, 276, 292, 293].

Material	Young's Modulus E (MPa)	Poisson's Ratio ν	Tensile Stress σ_{TS} (MPa)	Fracture Toughness K_{IC} (MPa·m ^{1/2})	Strain energy release rate G (J/m ²)	Mineral Density ρ (g/cm ³)
Steel	200000	0.3	-	-	-	-
Dentine	19800	0.31	70	3.15	110	-
Pulp	10	0.49	-	-	-	-
PDL	70.3	0.45	-	-	-	-
Bone	12200	0.26	-	-	-	-
Uniform Enamel	84,100	0.3	50	1.05	12.7	2.83
Outer enamel	84,100	0.3	50	0.67	4.86	2.83
Middle enamel	70,000	0.3	50	1.6	36.26	2.7
Inner enamel	60,000	0.3	50	2.5	94.80	2.65

The critical strain energy release rate G (J/m²) is a material parameter related to the fracture toughness K_{IC} (MPa·m^{1/2}), indicating the energy required to propagate unit area of a crack. For a 2D plane-strain model, strain energy release rate (G) can be calculated as follows:

$$G = \frac{K_{IC}^2}{E^*} \quad (3.1)$$

$$E^* = \frac{E}{1-\nu^2} \quad (3.2)$$

where E is the Young's modulus, ν is Poisson's ratio and K_{IC} is the fracture toughness of the material.

3.2.4 Extended finite element method (XFEM)

Fracture analysis signifies an important field in engineering and has gained growing popularity in dental materials and biomechanics research recently. Ichim et al. [294, 295] developed a 2D model for simulating the formation of dental abfraction lesions by using the continuum-to-discrete element method (CDEM). In a further study [296] they modelled crack initiation and propagation for a range of case scenarios, such as contact-induced damage in layered materials systems and the failure of enamel, dentine, restored tooth and all-ceramic dental bridges. Barani et al. [297, 298] investigated longitudinal cracking in enamel by XFEM, in which the simulated cracks were in agreement with the experimental observations of the crack growth in human teeth. Li et al. [299] compared the CDEM and XFEM for studying the fracture behaviors of all-ceramic dental prostheses, showing the cons and pros of each method.

In this present study, the XFEM fracture analysis was performed to evaluate the formation of cracks in the occlusal fissure area using Abaqus 6.14 (ABAQUS, Inc, Providence, RI). The cracking criterion used here was the maximum principal stress criterion as [300],

$$f^e = \frac{\sigma_1^e}{(\sigma_{max}^0)} \quad (3.3)$$

where σ_{max}^0 represents the allowable maximum principal stress of the materials (enamel and dentine), σ_1^e is the maximum principal stress in element (e) and f^e indicates the stress ratio, determining if cracking would initiate in the element. A crack was assumed to occur when the maximum principal stress exceeds the prescribed tensile strength of the material. The subsequent crack growth was based upon the strain energy release rate [301]. The cracking region was considered in both enamel and dentine in the XFEM models. Detailed background information about the mechanics of XFEM fracture analysis can be obtained from the literature [86, 302].

3.3 Results

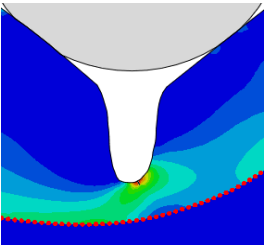
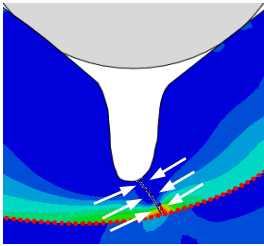
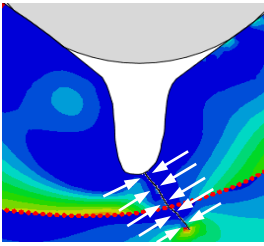
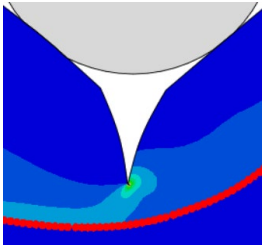
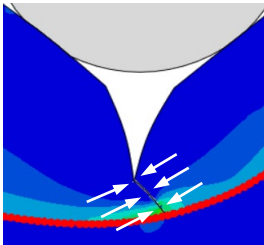
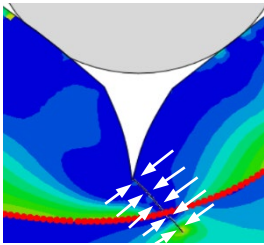
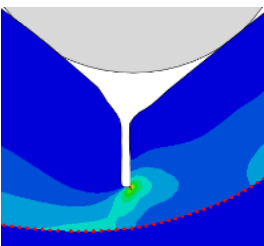
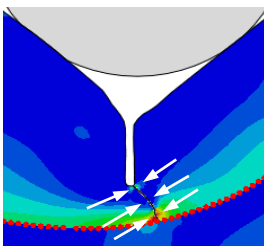
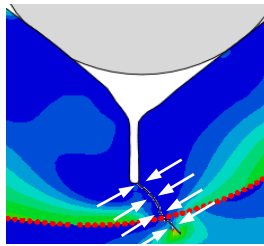
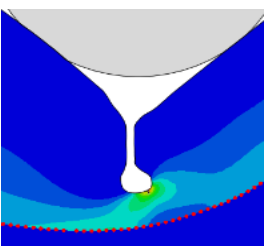
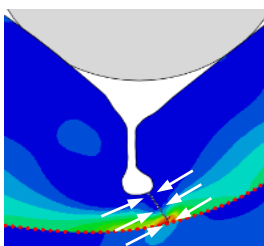
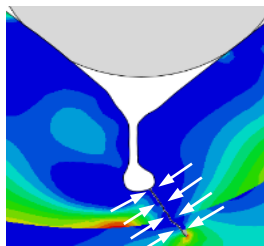
The influence of anatomical features and compositional factors, including fissure types, cusp angulation and material properties on the stress distribution, fracture load and crack length in the occlusal fissure of the tooth, are presented in the following sections.

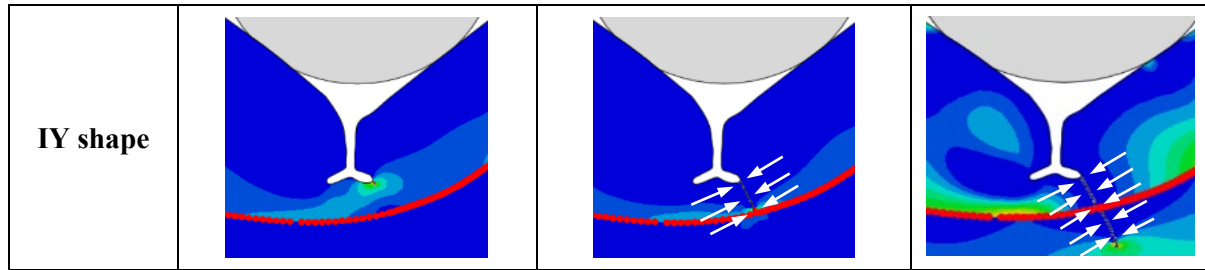
3.3.1 Fissure geometry

The contours of the maximum principal stress associated with crack initiation and propagation for the tooth models with the five types of fissure morphology at a cusp angle of 50° are shown in **Table 3.2**. The crack patterns at different stages of crack development, including crack initiation, crack growth to dentin-enamel junction (DEJ), and crack extension upon completion of indenter displacement loading, were recorded for these five fissure geometries. For all the fissure shapes, the crack generally started from the floor of the fissure where high tensile stresses occurred. Generally, the cracks initiated on one side of the fissure, and then propagated in the same direction. The cracks stopped growing once they reached the DEJ, which is marked as the red line in each sub-figure of **Table 3.2**. With continuation of

the loading, the crack passed through the DEJ and continued to grow in dentine. Consequently, the crack stopped in the dentine region when the displacement of the loading ball (0.2 mm) and the resultant loading was completed.

Table 3.2: Patterns of crack propagation for tooth models and the relevant maximum principal stress contour at different stages of crack formation including crack initiation, crack growth to DEJ and crack extension upon completion of loading. From top to bottom, the models have same cusp angle (50°), but different fissure geometries, including U, V, I, IK and IY shapes.

	Crack initiation	Crack growth to DEJ	Loading completion
U shape			
V shape			
I shape			
IK shape			



In the XFEM analysis, the reaction force of the loading sphere was recorded as the fracture load [303]. Thus, the loads corresponding to onset of the fissure crack are graphed in Figure 3.3. On the basis of the fracture loads at crack initiation, the U shape fissures showed the highest value, followed by the IK shape. The remaining three geometries (V shape, I shape and Inverted Y shape) presented lower but similar loads. Regarding the crack length, as shown by the grey bars in Figure 3.3, the longest extension was 1.25 mm which corresponds to the IY shape, followed by the V shape (1.12 mm), I shape (1.04 mm), IK shape (0.94 mm) and U shape (0.84 mm).

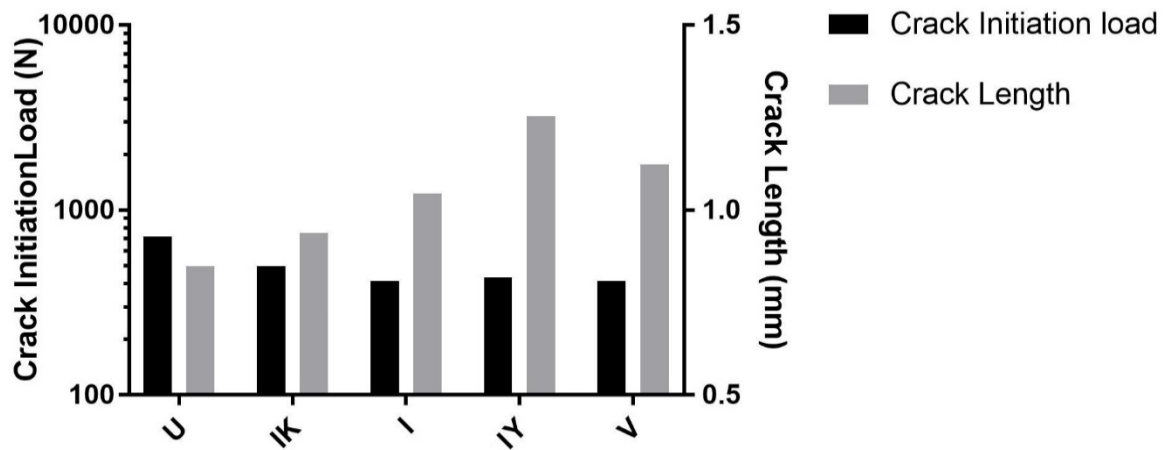


Figure 3.3: Crack initiation load (left Y axis) and crack length at completion of loading displacement (0.2mm) (right Y axis) for five fissure geometries, including U, IK, I, IY and V shape.

3.3.2 Cusp angle

The fracture loads at the onset of crack initiation were recorded from the XFEM analysis for different cusp angles (ranging from 50° to 70° at intervals of 2.5°) of each fissure geometry, as graphed in **Figure 3.4(a)**. It is observed that the fracture load rises with the increase in cusp angle (i.e. lower cusp steepness) for all fissure shapes. For the entire range of cusp angles, the U shape morphology resulted in the highest fracture load at crack initiation, followed by the IK shape. For the remaining three fissure types (V shape, I shape and IY shape), the fracture loads at crack initiation were similar, when cusp angle was at the low value of 50° (**Figure 3.4(a)**). Upon increasing the cusp angle up to 70° , the crack initiation load values for these three geometries were somewhat scattered with a decreasing rank of I to IY and V shape fissures.

By comparing the fracture initiation loads between the cusp angles of 50° and 70° , a relatively large difference was observed for the IK shape, I shape and IY shape (**Figure 3.4(a)**). For all the fissure geometries, the crack initiation load was relatively stable for the cusp angles between 50° and 57.5° ; and then increased for the cusp angles from 57.5° to 70° . Regarding the IK shape, the loads at crack initiation were fluctuating and increasing. For the I shape and IY shape, the loads fluctuated when the cusp angle was between 50° and 60° , and increased when the cusp angle was between 60° and 70° .

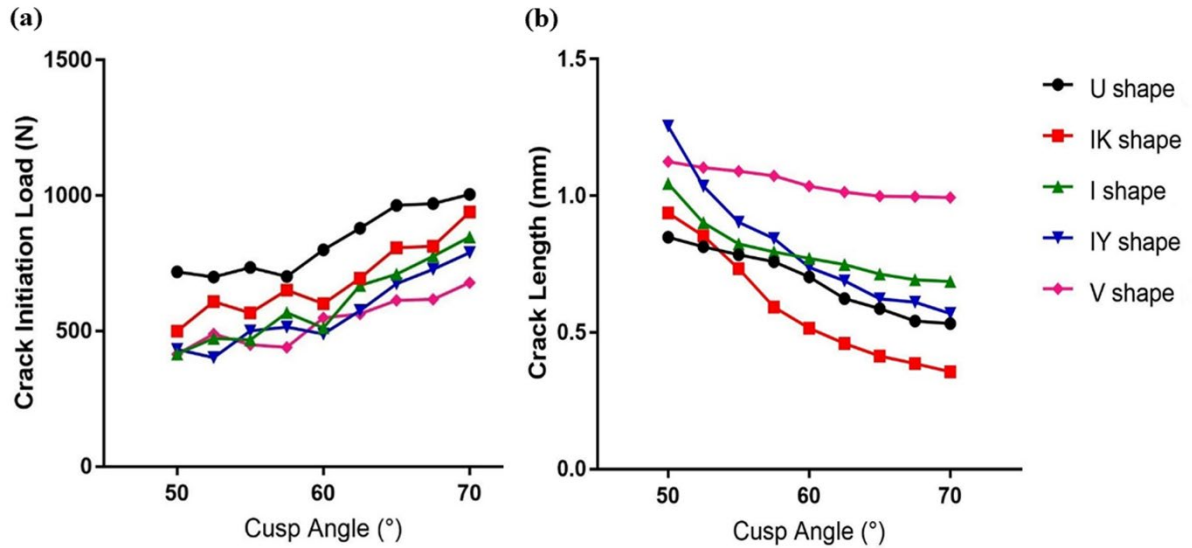


Figure 3.4: (a) Comparison of the fracture load at crack initiation; (b) Crack length at completion of loading, for the models with different fissure geometries and different cusp angles (from 50° to 70° in an interval of 2.5°)

Crack lengths and maximum load upon completion of the loading displacement were also recorded from the XFEM analysis for the different fissure geometries and various cusp angles (**Figure 3.4(b)**). Comparative results of the crack length among all five fissure shapes, for the cusp angle of 50°, are shown in **Figure 3.3**. **Figure 3.4(b)** graphs the crack length values upon completion of loading for different cusp angles (from 50° to 70°). Accordingly, the crack lengths decreased with the increase in cusp angle for all the fissure geometries. The V shape had the least change in the crack length for different cusp angles between 50° and 70°. The slope of decreasing trend of the U shape was greater than the V shape, which was fairly stable within the entire cusp angle range. The IY shape, I shape, and IK shape had a similar trend, i.e. crack lengths declined sharply when cusp angle changed from 50° to 57.5°, followed by a smaller rate of crack length reduction in the cusp angle range of 60° to 70°.

The reduction of the crack length was more significant in the IK and IY shape fissures, where the crack length almost halved when increasing the cusp angle from 50° to 70°. At the low cusp angle of 50°, the crack length of V shape fissures was significantly larger than those of the other fissure types which exhibited a decreasing rank of I shape, IY shape, U shape and IK shape.

3.2.3 Material properties of enamel

The fracture behavior of enamel in relation to the gradient of mineral density and corresponding material properties of enamel in different parts of the tooth including the fissure area were investigated for different fissure geometries. Accordingly, the fracture loads at different stages of crack formation were recorded for the models with constant material properties throughout the enamel as well as the models with an allocated CT-based gradient of material properties in enamel. **Figure 3.5** shows the comparative results of the fracture loads at crack initiation, crack growth to DEJ and upon completion of loading displacement for these models with the constant and graded material properties at a cusp angle of 50°. In general, the models with gradient of mineral density and graded material properties showed a trend of increased fracture loads in all three stages of crack formation in comparison with the similar models with constant mineral density. The effect of graded versus constant mineral density was more significant in the second stage of crack development (crack propagation to DEJ) compared with the crack initiation and maximum crack extension at the displacement completion stages. In the crack initiation and loading completion stages, none of the fissure geometries were overly sensitive to the changes in the mineral density, where both the constant and gradient density models had relatively close fracture loads. However, in the stage of crack growth to DEJ, the application of gradient density on the models, significantly

increased the load values for the U shape, V shape and I shape, to almost twice that of the models with constant density (**Figure 3.5**). The graded mineral density also resulted in an increase of the loads for crack growth to the DEJ in the IK shape and IY shape models, however the effect was relatively small compared to the other three geometries.

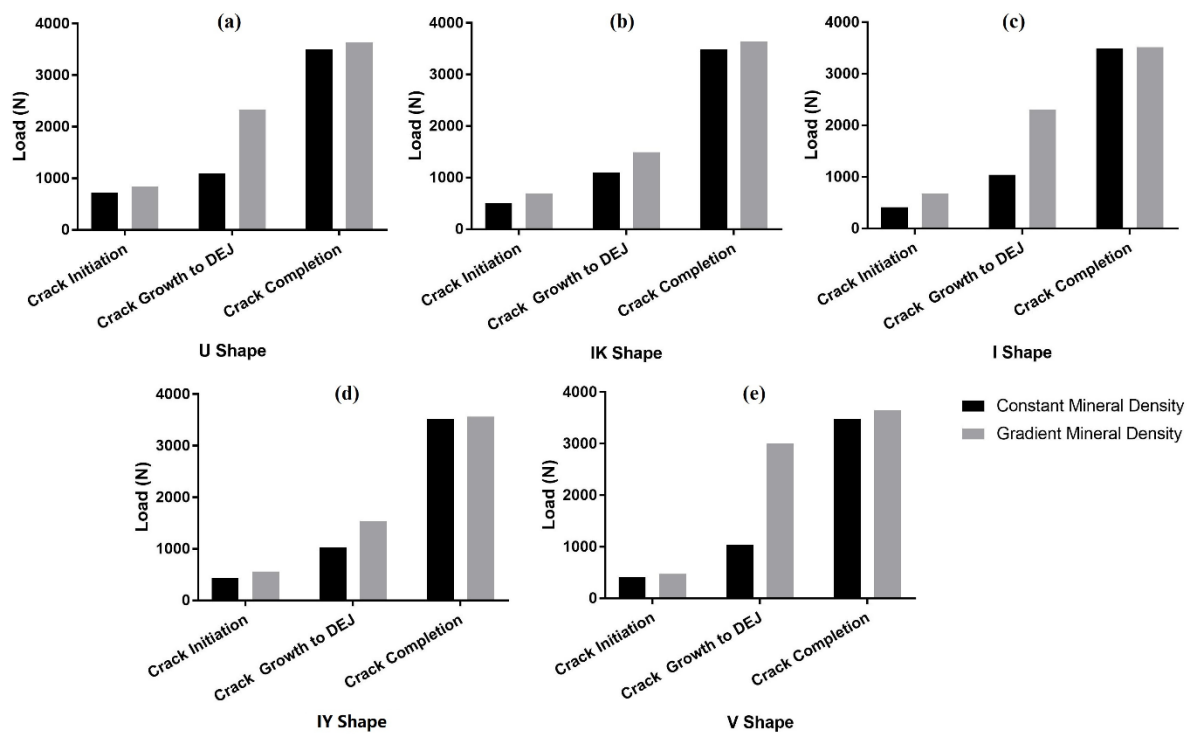


Figure 3.5: Fracture load at crack initiation, crack growth to DEJ and crack completion stages for the models with constant and graded mineral density and material properties at a cusp angle of 50°.

Further to investigate the combined effect of fissure geometry, cuspal angle and material properties of enamel on the fracture behaviour of occlusal fissures, the crack length at the completion of the loading displacement was recorded. **Figure 3.6** shows the comparative

results of the crack length for the different fissure types at cusp angles of 50°, 60° and 70° for the models with constant and graded mineral density. It was noted that the crack length in the models with graded mineral density was generally smaller than that in the constant density models regardless of cusp angle and fissure geometry.

At a low cusp angle of 50°, prescription of a CT-based gradient of mineral density had significant effect on the fracture resistance and led to a sizeable decrease in the crack length for all the fissure geometries. For both the gradient and constant mineral density patterns at 50° angle, the U shape geometry had the smallest crack length, followed by the IK shape, I shape and V shape. The IY shape demonstrated the most substantial crack length of all the fissure geometries, indicating lowest fracture resistance.

While the IY shape was the most affected geometry by the gradient mineral density at the low cusp angle of 50°, mineral density gradient did not have a significant influence on the crack length for the I shape and IK shape fissures at a cusp angle of 70°. In these fissure types, the effect of graded mineral density became smaller with increasing cusp angle from 50° to 70°. The influence of gradient density on the crack extension was evident in all cusp angle values for the U shape and V shape fissures.

At the high cusp angle of 70°, gradient mineral density led to smaller crack lengths for the U shape, V shape and IY shape. As for the IK shape and I shape, change in mineral density had limited effect on the crack length.

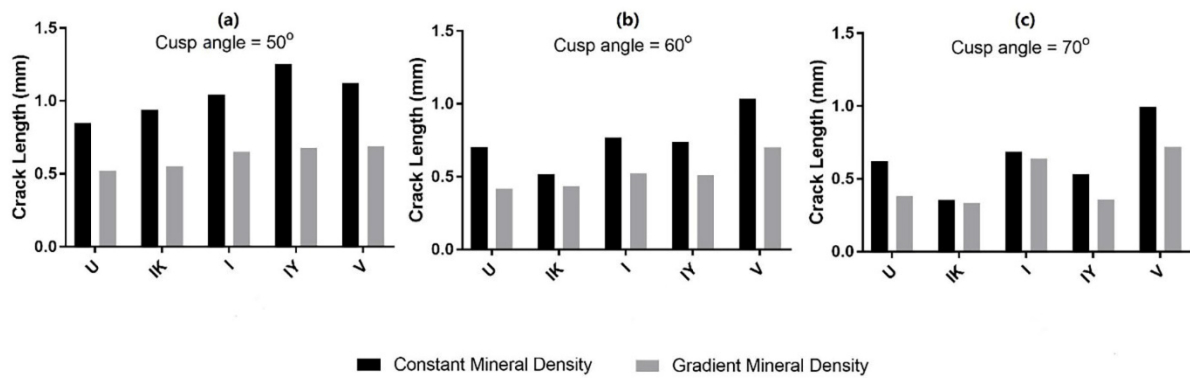


Figure 3.6: Crack length of the models with constant and graded mineral density for the different fissure types at cusp angles of 50°, 60° and 70°.

3.4 Discussion

Cracking and fracture of the tooth imposes a significant concern in the clinic, with a questionable prognosis for tooth fracture in majority of the patients [105]. This issue is more frequently diagnosed in teeth with deteriorated structural integrity due to caries or large intra-coronal restorations [304]. However, the rate of the fracture is very low in sound teeth despite the presence of deep fissures on the occlusal surface as well as thin brittle enamel in these areas of the tooth. In this study, we investigated the interaction of various anatomical features and compositional factors which contribute to the resistance of the fissural enamel against fracture.

As shown in **Table 3.2**, in all the study groups, the cracks initiated at the fissure area in which the maximum tensile stress was concentrated; and propagated toward the right lower direction in the enamel, presumably due to the non-symmetrical structure of the modelled tooth. The non-symmetrical anatomy of the models were created to reflect the structural

asymmetry of the natural premolar tooth in which the functional cusp is generally smaller and has a rounder shape in comparison with the sharper and larger non-functional cusp. The directional propagation of the crack toward the smaller cusp, can be attributed to smaller bulk of the enamel and dentine together with the lower thickness of enamel, which leads to higher stress concentration.

Regarding the effect of the geometry of the occlusal fissure on fracture resistance of the tooth, the results of the XFEM analysis showed that the fissures with larger curved morphology, such as U and IK shape, exhibited higher resistance to fracture under simulated occlusal load irrespective of cusp angle and enamel material properties. At the crack initiation stage, these two fissure types required higher fracture loads to generate the crack. This may be explained by their curved morphology that distributed the stress over a wider area and prevented stress concentration around localized points in the fissure. On the other hand, the I, IY and V shape fissures displayed similarly lower fracture loads and longer crack lengths at maximum load displacement due to their sharp and pointed shape at the tip of the fissure which prevented wider distribution of the stress and generated greater stress concentration.

The cusp angle is an important anatomical feature of the crown morphology which can be modified and adjusted in natural tooth and restorative crowns. Previous studies have evaluated the relation of cusp angle with the fracture resistance of ceramic crowns and the values between 50° and 70° have been suggested ^[284] to be an optimum range of cusp angle. However, to the knowledge of the authors, the effect of cusp angles in combination with the fissure morphology and gradient properties of natural teeth have not been investigated before.

As shown in **Figure 3.4(a)**, increasing the cusp angle (i.e. decreasing the cusp steepness) results in the increase of the fracture resistance of the tooth. This finding is consistent with

the mechanical test conducted on ceramic crowns by Sornsuwan et al. [305]. The applied occlusal force can be resolved into two components in the lateral and longitudinal (axial) directions. While higher cusp angulation is more related to the compressive stress and longitudinal (vertical) forces, steeper cusp inclination generates larger horizontal forces in the fissure area which is the dominant factor in crack initiation and propagation. In our study, the crack initiation load was almost unchanged for the cusp angles between 50° and 58° , and was sensitive to the cusp angle above 58° (**Figure 3.4(a)**). We assume that at the cusp angle values below 58° , the tensile stress caused by the horizontal force component is large enough to initiate and propagate the crack irrespective of the specific cusp angle for all the fissure geometries. However, the crack length at maximum displacement was still proportionate to the cusp angle value even in this low range of cusp angle values (**Figure 3.4(b)**).

Material properties play an important role in crack growth of the structures. While some studies have considered enamel as a homogenous material [306], others have suggested enamel to be a functionally graded material with a gradient of material properties [307], [308]. In the current study, we used non-destructive microCT imaging to obtain mineral density maps in various sections of the tooth and subsequently generated Young's modulus and fracture toughness maps of the specimen. Young's modulus is a critical material property which influences the stress and strain energy, thereby determining crack initiation and propagation.

Our XFEM method consisted of two stages; the first was crack initiation which simulated the crack nucleation and small crack growth; and the second stage modelled the propagation of the crack. Regarding the crack initiation, the materials with a lower modulus would allow more elastic deformation, i.e. more compliant (softer) [289]. Lower Young's

modulus will lead to a lower tensile stress of the material; and therefore it would be more difficult for the crack to initiate. For the crack propagation, the determinant factor is the strain energy release rate (G) [309], which is inversely proportional to Young's modulus and directly proportional to the fracture toughness squared (Eq. (3.2)). According to the mineral density maps of the tooth, enamel in the fissural region has a relatively lower Young's modulus and higher fracture toughness than the outer enamel area. As a result, the crack would be more difficult to initiate and it would propagate more slowly under loading displacement in the fissural area.

As shown in **Figure 3.5**, graded material properties had a more significant impact on the fracture load during the crack growth stage compared to the crack initiation and maximum crack extension stages. To explain this observation, we assume that for the models with graded properties in enamel, crack needs more load to grow across enamel before reaching the DEJ, as the strain energy release rate for functionally graded enamel is significantly higher than that of the models with homogenous constant properties. Regarding the load at crack completion, nevertheless, there was no significant difference in the fracture loads. This is due to the fact that the crack had already passed the DEJ and entered the dentine for both constant property and graded enamel property groups and therefore the crack opening displacement is controlled by the strain energy release rate of the dentine. The reduction of fracture load due to the graded material properties was more manifest for a lower cusp angle particularly in the fissures with V and I shape, where the increase of the cusp angle is not able to impart significant resistance against fracture loads.

As shown in **Figure 3.6**, if the cusp angle is in the lower range of the suggested values, graded material properties could be one of the ways to increase the resistance of the tooth to

crack growth. However, with the increase in cusp angle, the effect of material properties on crack length became smaller due to the lower tensile stress.

According to these findings, application of tougher materials around the occlusal grooves can be an effective strategy to lower the risk of fracture for the intra-coronal restoration or crowns under heavy masticatory loads when the cusp angle cannot be increased. Avoiding the creation of sharp and narrow morphological features on the occlusal surface of the restoration is also of utmost importance to the enhancement of durability and resistance of the tooth and restoration.

Based upon the findings of this study, we suggest three mechanisms have been incorporated into the natural design of the tooth endowing it with the maximum resistance against masticatory loads while still maintaining the benefits of a multicuspid dentition with narrow and deep occlusal fissures. The first mechanism is the rounding and radial extension of the fissure tip which allows more even distribution of the stresses over a larger area. The second mechanism involves the increase of the cusp angle (reduction of the cusp steepness) which has been adopted more significantly in highly load bearing molar teeth compared to premolars. Interestingly, the gradual wear and attrition of the occlusal surfaces in subjects with high masticatory load level, which leads to the increase of the cusp angles, can be considered as a protective mechanism that can reduce the risk of cracking and tooth fracture in these subjects.

Finally, the gradient of mineral density and material properties within enamel, i.e. higher toughness of inner and fissural enamel, provides a way to offset the destructive consequences of stress concentration caused by the sharp morphology around fissure tips. The collective effect of these anatomical and compositional features along with the intricate microstructural

properties such as hierarchy, remnant proteins, orientation and bundling of hydroxyapatite crystals makes enamel an extraordinary material with many unique properties.

3.5 Conclusion

This study investigated the fracture behavior of fissural dental enamel under simulated occlusal load in relation to various interacting factors including fissure morphology, cuspal angle and the underlying material properties of enamel. XFEM was adopted to analyze the fracture load and crack length in tooth models with different anatomical variables. Overall, the outcomes of this study explain how the interplay of compositional and structural features of enamel in the fissural area contribute to the resistance of the human tooth against masticatory forces. These findings may provide significant indicators for clinicians and technicians in designing/fabricating extra-coronal dental restorations and correcting the cuspal inclinations and contacts during clinical occlusal adjustment.

Chapter 4: Mechanical failure of posterior teeth due to caries and occlusal wear

Caries and wear are two tooth level conditions which have been commonly observed in cracked tooth. Caries is a plaque induced phenomenon which involves the dissolution of crystal structure of hydroxyapatite in enamel and dentine. Demineralized enamel displays higher porosity, decreased mineral concentration and diminished material properties. The purpose of the present work is to explore the effect of occlusal wear and different types and degrees of caries on the mechanical performance and structural integrity of posterior teeth. Presence of fissural caries, if not treated (either with remineralization, resin infiltration or restoration), can be a major risk factor in the initiation of tooth fracture. When combined with decreased enamel thickness and loss of proximal marginal ridge due to mechanical or chemical wear, the weakening effect of the caries will be amplified specially in teeth with steep cuspal slopes. The application of a conservative treatment with resin infiltration can be an effective approach in prevention of further mechanical failure of demineralized enamel. The findings of this study emphasize the importance of early interventions in the management of caries for the prevention of future cuspal or tooth fracture especially in subjects with higher risk factors for tooth fracture such as caries, wear and bruxism.

4.1 Introduction

Teeth are unique biological structures naturally designed to last for a lifetime, therefore humans grow no new teeth after the complete eruption of their permanent dentition. It is the ingenious combination of smart structural configuration with optimized material properties of

enamel, dentin and their sophisticated junction which has endowed teeth with outstanding resistance against millions of cycles of masticatory loading [310]. While understanding the remarkable resistance of the tooth and the role of its building blocks have been the research foci of many contemporary studies, the increasing incidence of tooth cracks and fractures in recent years has posed significant questions and challenges for both the patients and clinicians.

Teeth with cracks have become a common occurrence in adults, with prevalence rates of up to 70%, and the problems associated to cracked teeth are the third leading cause of tooth loss after caries and periodontal disease [311]. The increasing incidence of tooth fractures in the modern age can be partly attributed to the widespread iatrogenic damage caused during the preparation of the restoration cavities according to the principles suggested by G.V. Black in the last century [312]. Inappropriate cavity design, introduction of stress concentration sites within the tooth structure and insufficient remaining structure of the natural tooth tissue are some factors that play a certain role in weakening of the restored tooth structure and deterioration of its mechanical integrity. Other contributing factors such as unusual mechanical loading (i.e. acute forces in trauma or chronic forces in bruxism), aging, fatigue and endodontic treatment have also been suggested to increase the fracture susceptibility of teeth [311].

On the other hand, cracking and fracture have also been reported in intact teeth with no preparation and restoration, though to a lesser extent [313]. Some researchers have investigated the role of anatomical variations and aging on the fracture resistance of intact teeth [109, 314-317]. However, the additional roles of caries and wear, which can significantly alter the local composition and micro/macro structure of enamel and dentine,

have not been studied in detail. Understanding the mechanical failure of prepared and restored teeth deserves an extensive study on various cavity preparation parameters and therefore remains out of the scope of the current work which mainly focuses on the fracture in non-restored and non-cavitated teeth.

Caries and wear are two tooth level conditions which have been commonly observed in cracked teeth [318]. Caries is a plaque induced phenomenon which involves the dissolution of the crystal structure of hydroxyapatite in enamel and dentine. Demineralized enamel displays higher porosity, decreased mineral concentration and diminished material properties [319]. In caries affected dentine, although the mineral density and mechanical properties are decreased compared to sound dentine, a layer of reactionary dentine can form around the pulp area and beneath the caries location, resulting in the shrinkage of the dental pulp and reduction of its volume [320]. The extreme manifestation of caries activity is the fracture and destruction of the caries affected areas and formation of a cavity which can further extend to involve and undermine the entire cusp of the tooth.

Tooth wear, which progressively modifies the morphology and occlusal loading condition of the tooth [321, 322], is not only a common observation in cracked teeth but also an indication of prolonged and heavy biting forces in the individual. The clinical manifestations of wear include the reduction of the cuspal slope, decreased enamel thickness and weakening or loss of the proximal marginal ridge of the tooth [321]. Different types of tooth are categorized based upon the dominant etiological factors which include chemical (erosion) or mechanical (attrition, abrasion and abfraction), though a combination of both mechanical and chemical factors are generally considered to be involved in extensive wear cases (for example in a bruxer patient with gastric reflux) [321]. Whether the wear is a

coexisting presentation or a causative factor in the formation of dental cracks remains an open research question.

Despite the increasing incidence of dental cracks, there is no consensus among clinicians regarding the causes, prevention methods and treatment protocols for the affected teeth. Understanding the key causative factors responsible for the initiation and progression of cracks in individuals and for a specific tooth is of great significance for fracture risk assessment and development of preventative and treatment protocols for clinicians. One of the major challenges for the experimental study of the fracture process in human teeth is obtaining minimally destructed samples with little variation in the size, morphology and material properties. Simulation methods such as finite element analysis (FEA) and extended finite element method (XFEM) have proven to be a valid alternative approach for the analysis of the stress distribution, crack initiation and fracture pattern of three-dimensional models. FEA and XFEM have been employed in dental research for a variety of materials and case scenarios such as the contact-induced damage in layered materials systems and the failure of enamel, dentine, restored teeth and ceramic crowns. [106, 109, 323, 324]

Therefore, the purpose of the present work was to explore the effect of various consequences of caries and wear conditions on the mechanical performance and structural integrity of posterior teeth through the extended finite element method (XFEM). In addition, the effect of a conservative non-operative treatment using resin infiltration on the recovery of mechanical properties of carious teeth was assessed.

4.2 Methods and materials

4.2.1 Finite element models

Computed tomography (CT) images of an extracted human lower molar tooth were employed to develop the first molar model. The geometry of the enamel, dentine and pulp were segmented using ScanIP (Simpleware Pty. Ltd, UK) and the surface refinement for each component of the tooth model was carried out. The resultant finite element (FE) model was exported as an IGES file to SolidWorks (SolidWorks Corp., USA) for further modification. The periodontal ligament (PDL) was created by offsetting (0.2 mm) the outer surface of the tooth root section, and the alveolar bone model was developed around the tooth roots [105, 325]. The base model (**Figure 4.1(a)**) was further modified in order to investigate two sets of clinical parameters regarding caries and tooth wear.

To investigate the effect of wear process in the fracture resistance of the teeth, three parameters were considered which include the marginal ridge presence, cusp angle and overall enamel thickness. The marginal ridge was selected as the geometrical parameter; therefore, two models: (i) without marginal ridge, and (ii) with marginal ridge, were built as shown in **Figure 4.1(b)**. Two cusp angles (50° as a steep versus 70° as a flatter cusp angle) and two enamel thicknesses (normal thickness with an average thickness of 1.5 mm versus worn enamel with an average of 0.75 mm) were also examined as the wear related parameters affecting the mechanical behaviour of the tooth.

To explore the role of caries in the fracture resistance of the teeth, two basic types of caries including fissure caries and adjacent caries were considered in this work (**Figure 4.1(c)**). In addition, a third group with combined fissure and adjacent caries was developed as

well. For each caries type, four lesion sizes were examined, i.e. small, medium, large and connected lesions. Accordingly, small caries spanned half the enamel thickness, medium caries extended up to the dentine-enamel junction, and large caries extended into the dentine. In addition, models with shrunk pulp size were developed to address the effect of caries progression and the subsequent pulpal shrinkage on the fracture strength of the teeth.

Further analysis of the effect of resin infiltration treatment on the cracking initiation load and final fracture load of the caries models was performed by assigning relevant material property values to the treated carious enamel of the corresponding models. It was assumed that the superficial etching treatment of the carious enamel which is usually performed before the application of the resin, did not significantly alter the material properties of enamel and the applied resin could well penetrate within the porosities of the treated carious lesion.

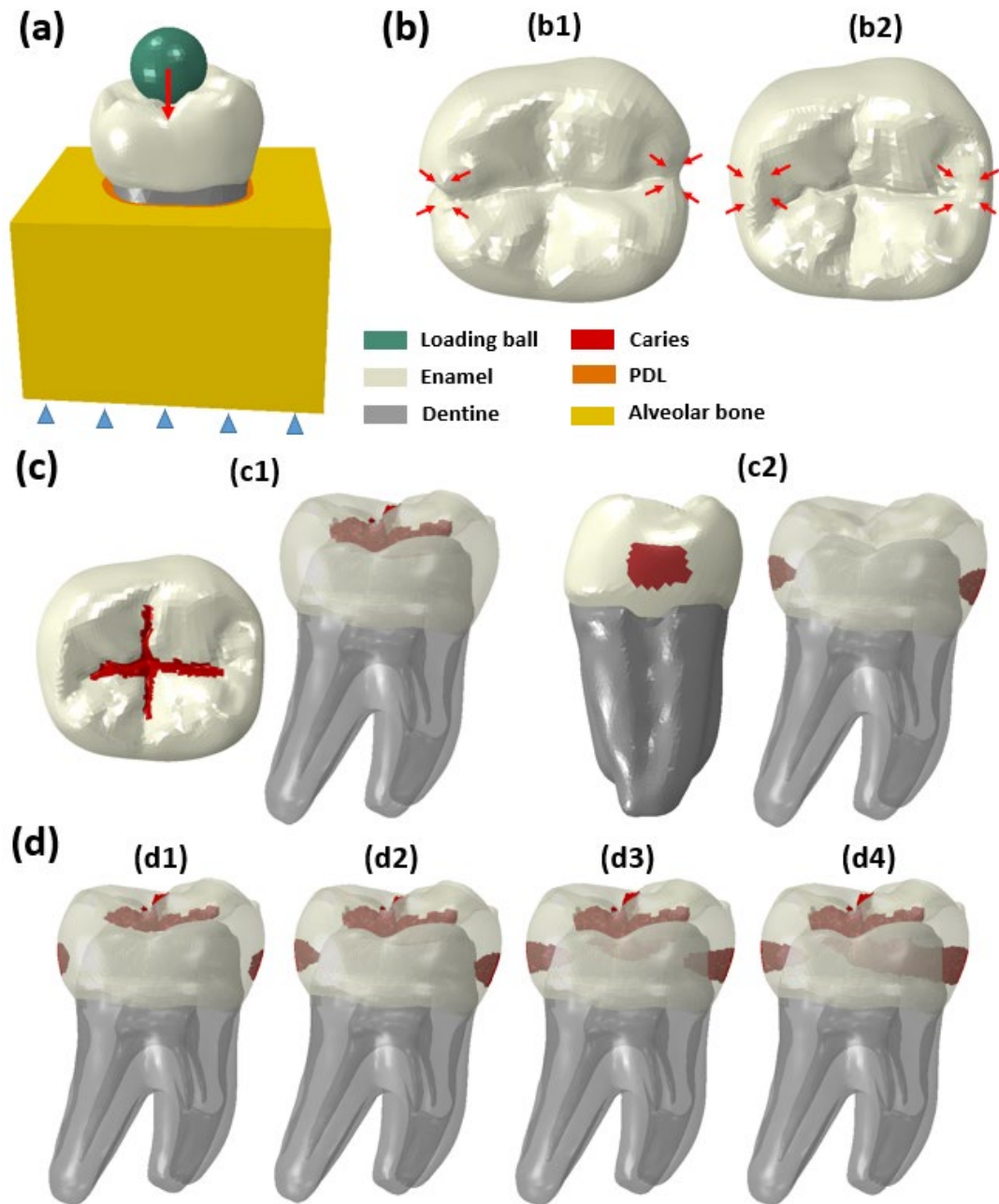


Figure 4.1: 3D finite element models for molar teeth. (a) the assembled finite element model consisting of the loading ball, enamel, dentine, PDL, and alveolar bone block. (b) two candidate geometrical parameters including (b1) model without marginal ridge and (b2) model with marginal ridge. (c) the tooth with caries lesion, (c1) fissure caries and (c2) proximal caries. (d) the representative model (combined caries) with various lesion size, (d1)

small size, (d2) middle size, (d3) large size, and (d4) connected caries, which is the limiting case in large lesion group.

The 3D FE models were meshed using four-node tetrahedron elements. A sensitivity analysis of the mesh was carried out to determine the appropriate mesh size. This step was performed to avoid the excessive computational cost and at the same time, to ensure the adequate accuracy of the simulation results. According to the sensitivity tests, the global mesh size was 0.5 mm for the whole model. Since the crack site would occur in the enamel and dentine region, a refined mesh with an element size of 0.3 mm was used in these two regions to obtain more accurate results. Consequently, the corresponding number of elements was 529,187 (Degree of Freedom - DOF: 289,515) for the tooth model, 347,346 (DOF: 189,666) for the PDL and alveolar bone, and 4,680 (DOF: 3,033) for the loading ball.

4.2.2 Loading and boundary conditions

According to the literature, direct application of the forces on the occlusal surface can lead to excessive stress around the loading area and further affect crack formation [326]. Therefore, in the present study, the tooth model was loaded using a 5mm ball controlled by a 0.3mm downward displacement. The contact between the loading ball and occlusal surface had a frictional coefficient of 0.3 [327]. The outer and bottom surfaces of the alveolar bone were kinematically constrained [328] as shown in **Figure 4.1(a)**. The interfaces between different tissues, including enamel, dentine, PDL, and alveolar bone were treated as perfectly bonded [286, 329].

4.2.3 Material properties

The loading ball was treated as steel [103] and each individual component was modelled as a homogenous, isotropic and linear elastic material for the stress and fracture analysis in this study [294, 296]. The required material properties were taken from the existing literature as summarized in **Table 4.1**.

Table 4.1: Material properties of the components of the FE model, adopted from the literature [103, 330].

Materials	Young's Modulus E (GPa)	Poisson's Ratio ν	Tensile Strength σ_{TS} (MPa)	Fracture Toughness K_{IC} (MPa·m ^{1/2})
Sound Enamel	84.1	0.3	50	0.86
Caries Enamel	10	0.35	8	0.22
Resin-infiltrated Enamel	12.5	0.3	15	0.32
Dentine	19.8	0.31	70	1.79
PDL	0.07	0.45	-	-
Bone	12.2	0.26	-	-
Ball	210	0.3	-	-

4.2.4 XFEM modelling

Different numerical models, such as cohesive zone [331], continuous-discrete elements [294, 296] and phase field [116] have been used for simulating fracture in different dental scenarios. In the present study, all the numerical analyses were performed using eXtended Finite Element Method (XFEM) in Abaqus 6.14 (ABAQUS, Inc, Providence, RI) which

allows simulating the crack initiation and propagation without mesh dependence and pre-defined path/region [5,15,22,28,30]. In the XFEM simulation, the maximum principal stress criterion was chosen as the fracture criterion [296, 332], and it can be represented as in Equation (4.1),

$$f^e = \frac{\sigma_1^e}{(\sigma_{max}^0)} \quad (4.1)$$

where σ_{max}^0 refers to the maximum allowable principal stress (tensile strength), σ_1^e is the maximum principal stress in element (e), and f^e represents the stress ratio, which determines if cracking will initiate in the element. A crack was assumed to occur when the maximum principal stress exceeded the pre-defined tensile strength of the material.

The subsequent crack extension should be perpendicular to the direction of the maximum principal stress. The energy based damage evolution criterion was adopted in this study [105], and it can be defined as a function of the crack initiation mix-mode [301], shown as Equation (4.2),

$$\left(\frac{G_I}{G_{IC}}\right)^\alpha + \left(\frac{G_{II}}{G_{IIC}}\right)^\alpha + \left(\frac{G_{III}}{G_{IIIC}}\right)^\alpha = 1 \quad (4.2)$$

where α is the power coefficient, and it can be taken as 1 [101, 301]. G_I , G_{II} , and G_{III} represents the strain energy release rates of crack extension in modes I, II and III, respectively. G_{IC} , G_{IIC} , and G_{IIIC} are predefined critical energy release rates at modes I, II and III, respectively. They can be calculated using Equations (4.3) and (4.4),

$$G_{IC} = \frac{K_{Ic}^2(1-\nu^2)}{E} \quad (4.3)$$

$$G_{IIc} = G_{IIIc} = \frac{1}{3}G_{Ic} \quad (4.4)$$

where K_{Ic} is fracture toughness, E is Young's modulus, and ν is Poisson's ratio.

4.3 Results

4.3.1 Crack patterns

Figure 4.2 compares the stress distribution contours at the crack formation state, the crack origin sites and final fracture patterns for the models with two different marginal ridge features. The maximum principal stress (MPS) contours were extracted when the crack initiated in the models. In the MPS contours (**Figure 4.2** (a1) and (b1)), the blue regions indicate compressive stress corresponding to the loading sites; and the red regions specify high tensile stress concentration. For both the models with and without marginal ridge, the stress distribution contours were generally similar, except for the extension of the stress areas along the mesial part of the occlusal fissure to the side of the tooth in the models with no marginal ridge (**Figure 4.2** (a1) and (b1)). In these models, the fissural areas in the mesial groove present the peak MPS values, in which the tooth exhibited a higher MPS value (63.5MPa) compared with the model with marginal ridge (51.9MPa).

Regarding the cracking patterns, **Figure 4.2** (a2) and (b2) show that the cracks originated at the base of the occlusal fissure regardless of the presence of the marginal ridge. The coronal view of the final fracture patterns in **Figure 4.2** (a3) and (b3) indicate that in the models with no marginal ridge, the crack extended uniformly along the mesial-distal fissure; while in the models with marginal ridge, the crack path was not uniform, where the crack grew from mesial fissure in the disto-buccal directions. In addition, the crack depth was not

even in the mesial-distal plane and it tended to spread more in the mesial side due to the steeper cusps and deeper occlusal fissures (isometric view in **Figure 4.2** (a3) and (b3)).

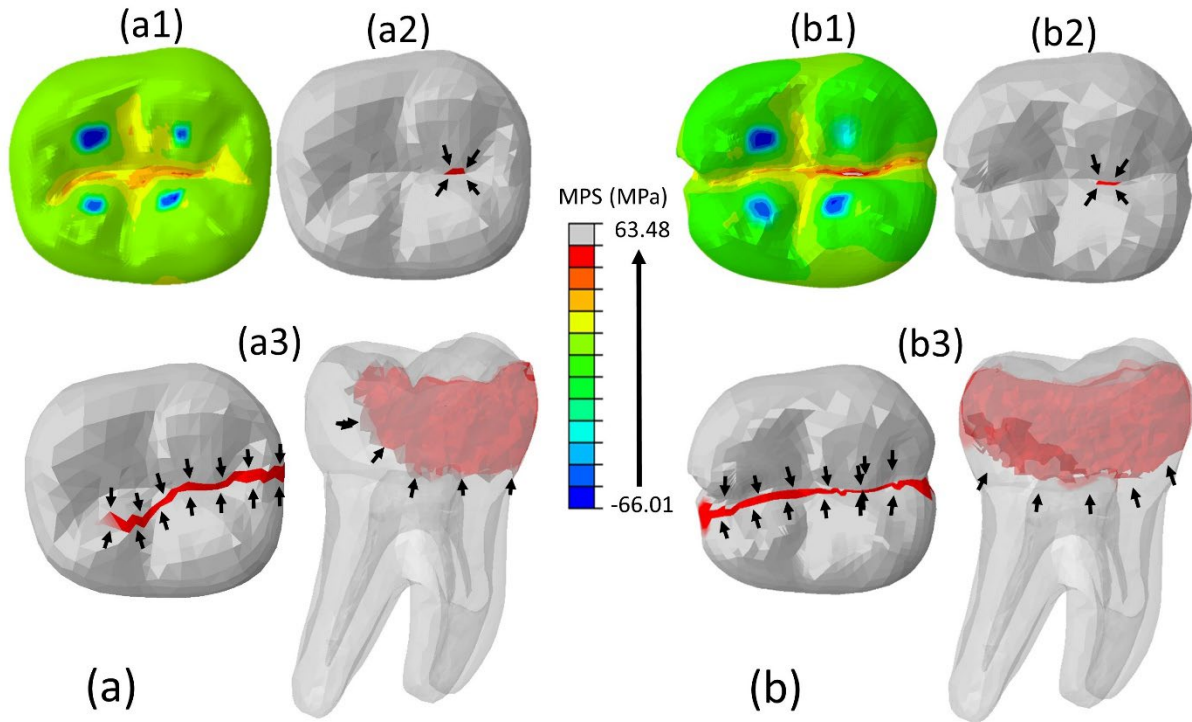


Figure 4.2: Maximum principal stress (MPS) contour in the crack formation state (a1 and b1), the fracture path including the crack origin site (a2 and b2) and final fracture pattern (a3 and b3) in the models. (a) with marginal ridge, and (b) without marginal ridge.

4.3.2 Crack initiation load and fracture load

In the XFEM analysis, the reaction force from the loading ball was determined, and the critical loads to initiate the crack were obtained from those different models (**Figure 4.3**). It was found that the absence or wear of the marginal ridge had a significant effect on the crack initiation load value. Accordingly, the groups with sound proximal marginal ridge generally exhibited higher load values, regardless of caries presence, size, and location. In fact, the

to wear process. However, the crack initiation load was not further decreased evidently with fissural caries size from small to moderate and even large (**Figure 4.3**). While the presence of fissure caries resulted in the substantial decrease in the crack initiation load values, proximal caries imparted little effect on the crack initiation load when compared to sound teeth.

To further analyze the fracture behavior of the models, their fracture load was further extracted once the crack reached the upper boundary of the dental pulp. **Figure 4.4** graphs the fracture loads in relation to the caries and marginal ridge parameters. In general, the presence of caries (either fissural or proximal) resulted in lower fracture loads, and a declining trend in fracture load with increase of the caries size. Although the effect of both the proximal and fissural caries on the fracture load value was minimal in small lesions, the medium and large fissure caries and combined caries models exhibited significantly lower fracture loads compared to the non-carious counterparts (**Figure 4.4**). The reduction of the fracture load was not significant in the models with proximal caries except for the models with large proximal lesions that presented a substantial reduction in fracture loads. Similarly, the groups with combined and connected large fissural and proximal lesions experienced the largest drop in the fracture loads compared to the sound tooth models. Accordingly, the effect of lesion location became evident only with the increase in the size of the lesion. For example, while a non-carious tooth with the marginal ridge showed a fracture load of 689N, a similar model with a large adjacent caries exhibited a fracture load of 603N followed by the models with fissure caries (397N), combined caries (366N), and connected combined caries models (295N), respectively.

Similar to the crack initiation load, the models with a marginal ridge exhibited a higher fracture load compared to those with no marginal ridge (**Figure 4.4**) for all the study groups.

Considering the collective effect of caries and marginal ridge on the fracture resistance of the tooth, the simulation results revealed that the models without marginal ridge exhibit a more significant reduction in fracture load due to the presence of the adjacent and combined caries, compared to the models with the same caries size and location but with a marginal ridge. In the worst condition of having two connected large proximal and fissural caries with no proximal marginal ridge, the fracture load dramatically dropped to only 25% of the load values in the corresponding sound model with a marginal ridge.

(normal versus shrunk) and different caries locations (proximal, fissure and combined).

Figure 4.5 (b) shows the final fracture pattern for the two representative models with the same occlusal features but different pulp sizes (normal versus shrunk pulp). Apparently, the shrinkage of the pulp size resulted in fracture load values to increase for both the carious and sound models. This increase was evident in all types of caries and was not affected by the location of the lesion. However, the final fracture pattern was similar for both the normal size and shrunk pulp groups (**Figure 4.5** (b)).

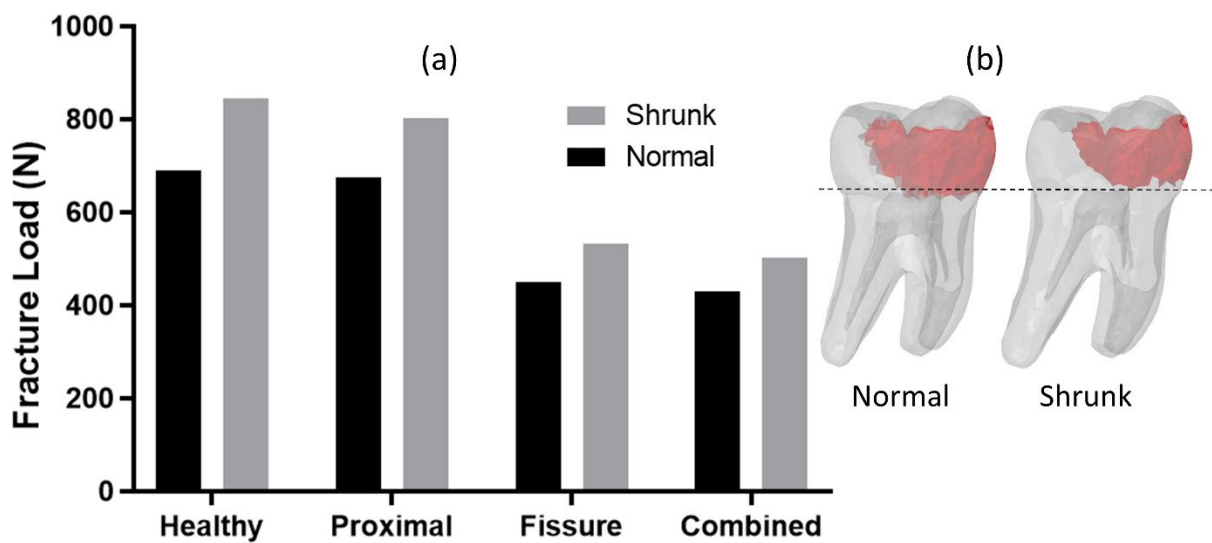


Figure 4.5: (a) Fracture load for the tooth models with different pulp sizes (normal versus shrunk) and caries locations (proximal, fissure and combined medium size lesions). (b) final fracture pattern in the representative models (normal versus shrunk pulp).

Figure 4.6 shows the comparative results of the crack initiation and fracture loads for the carious teeth and the teeth with resin infiltration treatment. Following the resin infiltration of the models with carious lesion, both crack initiation load and fracture load values increased significantly, regardless of the presence or absence of the marginal ridge. Furthermore, the increase in the crack initiation load (approximately 100%) was more prominent compared to

the increase in the fracture load (approximately 40%). By comparing the resultant values in **Figure 4.6** (a) and (b), it can be found that the models without marginal ridge were more affected by resin infiltration treatment in comparison with the corresponding sound models. Following the resin infiltration treatment, the fracture load values could recover up to 90% of the corresponding values for the healthy teeth, however, the crack initiation load could only recover to around 75% of the healthy tooth.

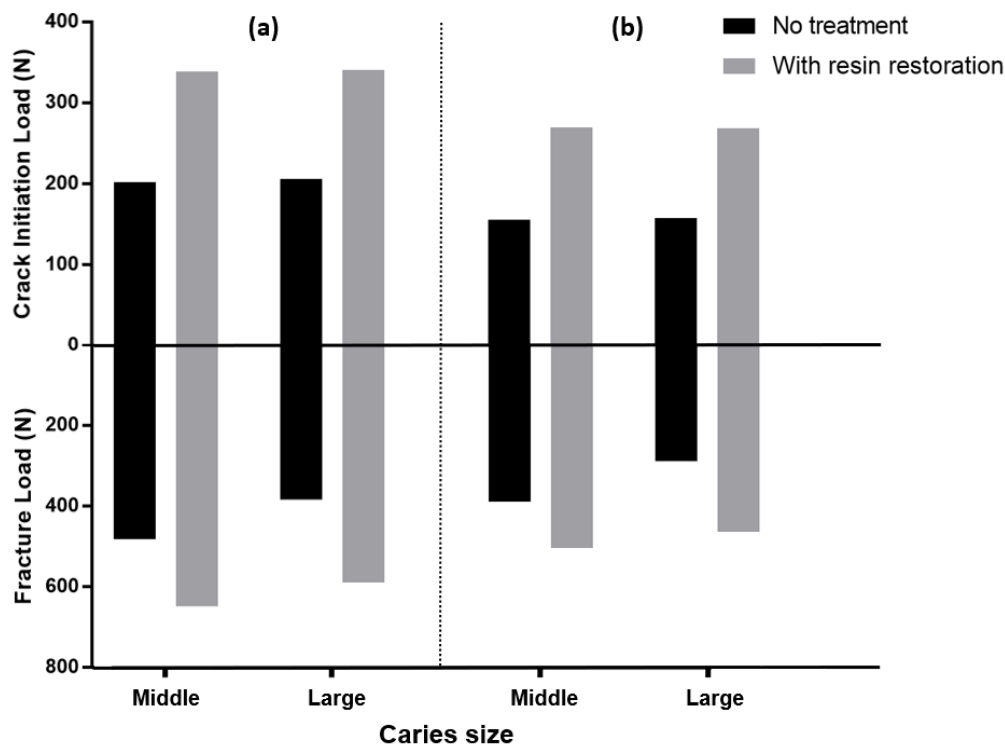


Figure 4.6: Crack initiation load and fracture load of the carious teeth with and without resin infiltration. (a) the models with marginal ridge. (b) the models without marginal ridge.

4.3.3 Force-displacement response

Figure 4.7 illustrates the force versus displacement curve for a representative model (deep fissure caries, with marginal ridge, normal enamel thickness and 50° cusp angle). With

the gradual increase of the applied force, several small load drops were observed which indicate step wise propagation of the crack.

During the simulation, the representative crack growth path was captured as displayed in **Figure 4.7**. According to the XFEM results, the crack origin and propagation path were not affected by the change in geometrical features of the occlusal surface, pulp size, as well as enamel material properties (caries effects). For all the tooth models, the crack initiation site was in the mesial portion of the occlusal fissure (**Figure 4.7 (i)**), where the cuspal slopes were steeper and the MPS value was the highest. The crack then propagated along the mesial-distal groove and downwards through the enamel until it reached the dentine enamel junction (DEJ) (**Figure 4.7 (ii) and (iii)**). Note that the crack appears to be arrested by the DEJ but continues to grow in the enamel on the side of the tooth to the cementum enamel junction CEJ before extending into the dentine. After the crack extended through the entire thickness of enamel, it grew into the dentine region progressively (**Figure 4.7 (iv)**) and finally stopped when reaching the pulpal space (**Figure 4.7 (v)**).

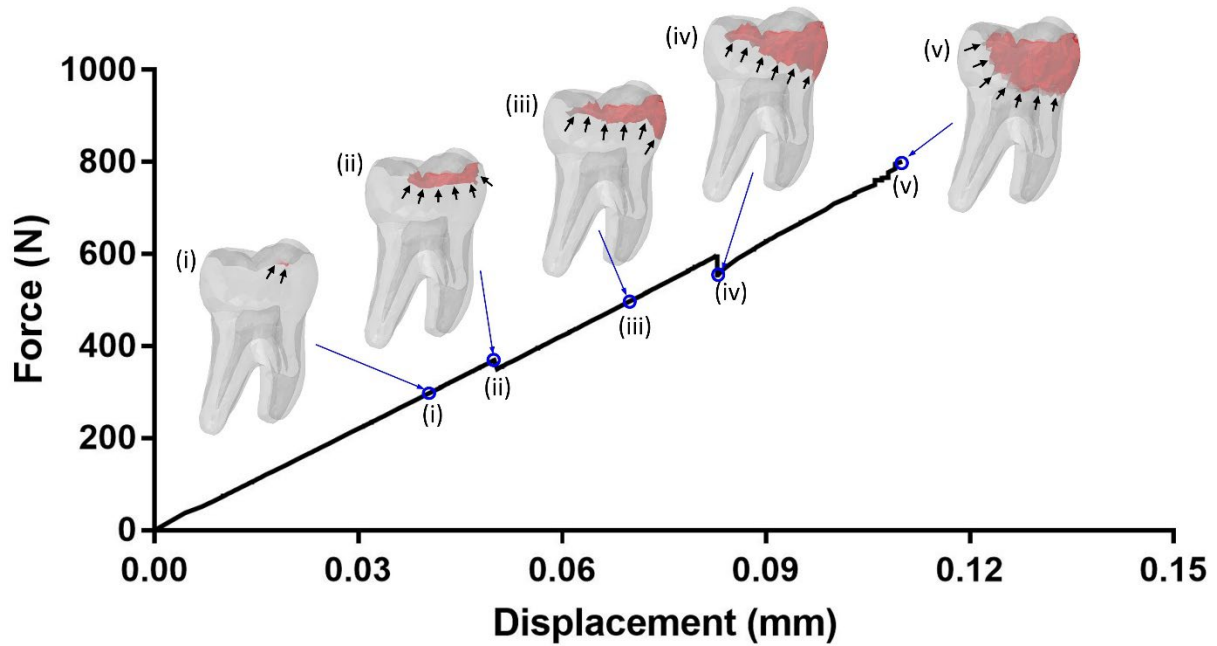


Figure 4.7: The force versus displacement curve along with crack growth pattern at various stages of loading in the representative model (healthy tooth with marginal ridge)

4.4 Discussion

Small cracks are a common observation in permanent teeth. While most of these cracks remain stable and asymptomatic for the entire life of the individual, in some cases the gradual propagation of the crack leads to pain and discomfort for the patient and can finally result in the catastrophic fracture of the tooth. Cracks are also a potential entry point for bacteria accessing the dentine pulp complex and causing pulp and peri-radicular diseases [333]. According to prevalence studies, fractures are mostly found in posterior teeth especially mandibular molars, which are the most commonly fractured teeth followed by maxillary molars with almost half the rate of crack incidence compared to mandibular molars [318]. Therefore, in the current study, a mandibular molar model was developed and XFEM was employed to identify possible risk factors at the tooth level which potentially predispose the

tooth for crack formation and tooth fracture. The studied factors were limited to caries and wear related parameters in unrestored and non-cavitated tooth models.

Recent data from a large number of dental practices have shown a significant correlation between caries and radiographic evidence of a crack and pain in cracked teeth [334, 335]. Experimental studies have also demonstrated the increased and accelerated fatigue and loss of mechanical strength in lactic acid and biofilm challenged dental tissues [336, 337]. On the other hand, dissolution of enamel has been shown to increase significantly in sites subjected to tensile loading [338], therefore creating a synergistic effect between caries demineralization and mechanical degradation of the tooth structure. In the current study, fissural caries and enamel demineralization at the base of the occlusal fissure were found to have a significant role in the initiation of the occlusal crack and reduction in the mechanical strength of the tooth. Fissural caries and associated cracks may not be visible in clinical examination or conventional X-ray images. However, instances of fine cracks originating in carious lesions can be observed using high resolution micro-CT images (**Figure 4.8**).

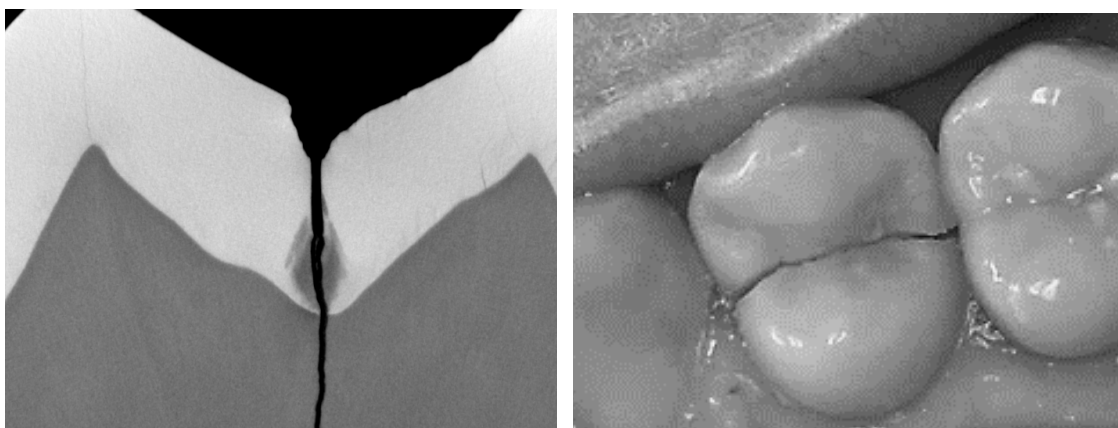


Figure 4.8: (a) micro-CT image of a lower molar tooth showing the presence of fissural caries and an associated crack originating from the carious fissure. (b) split fracture of an intact upper premolar tooth.

The decreased mechanical strength of carious fissural enamel (due to increased porosity and acid induced crystal defects), when coupled with increased cuspal flexure due to the absence of the marginal ridge was identified as a significant cause for crack initiation. Although, proximal carious lesions didn't have a significant effect on the initiation of the crack in the loaded models, they could facilitate further propagation of the initiated crack when having a large size and extending into dentine. On the other hand, the shrinkage of the dental pulp due to the formation of the reparative dentine which usually forms in chronic caries [320], was shown not only to have a protective role for the pulp, but also to potentially enhance the overall fracture resistance of the tooth, thereby compensating the loss of the mechanical strength due to demineralization activity. It should be noted that in the current study the values used for the mechanical properties of the dentine (Young's Modulus and Poisson's Ratio) were an average representative of various measurements from different teeth and different areas of the dentine. These values may display some variations between sound dentine and reactionary dentine which is formed around the pulpal area.

In addition to the role of marginal ridge, the effect of wear related cusp angle and enamel thickness reduction were evaluated in simplified 2D models (**Figure 4.9 (a)**). For the normal tooth model, a cusp angle of 50° and an average thickness of 1.8 mm were assigned for the occlusal enamel. Two models with a flattened cusp angle (70°) and reduced enamel thickness (0.7 mm) due to wear process were also developed and analyzed respectively. As shown in **Figure 4.9 (b)**, a flattened cusp angle resulted in the increase of both the crack initiation load and the fracture load values; however, thinner enamel thickness led to the significant reduction in the load values. In fact, the reduced cuspal steepness due to wear process,

seemed to play a compensating protective role against dental fracture and create an adapting response to the applied heavy occlusal loading.

Regarding the fracture pattern, although the crack propagation paths were generally the same for the selected models, the crack origin for the flatter cusp angle model was found to occur around the loading area, compared to the other two groups where the cracks originated from the base of the central fissure.

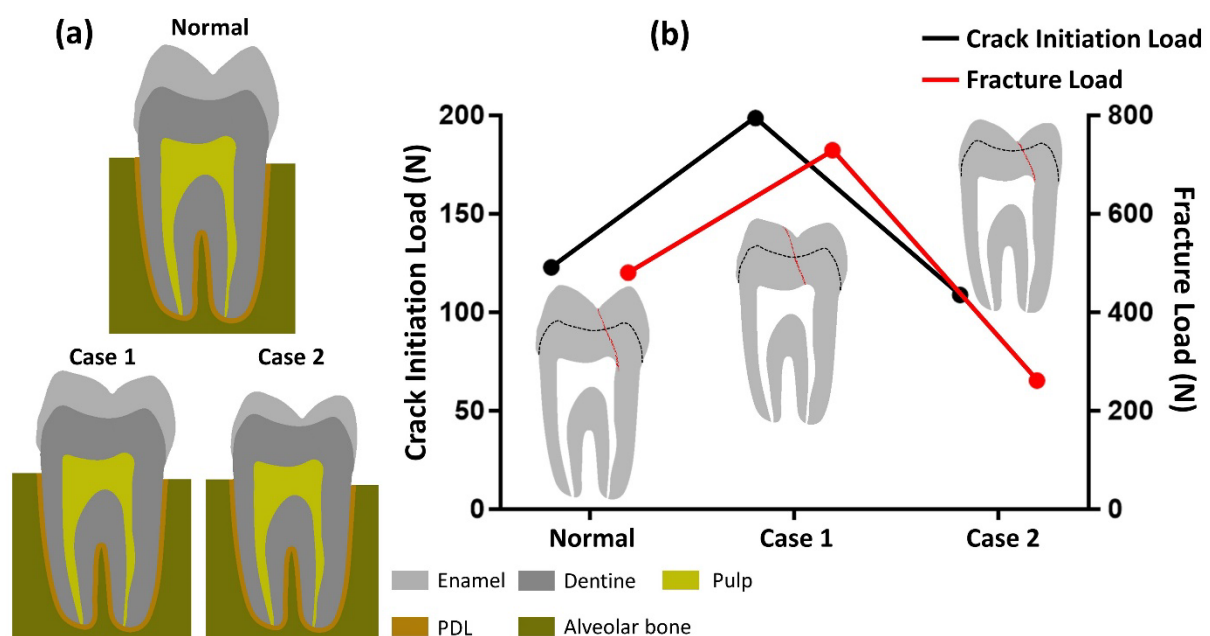


Figure 4.9: (a) the simplified 2D tooth models. Normal tooth indicates the intact tooth. Case 1 and Case 2 show the two representative examples without occlusal wear (average thickness of 1.8 mm of occlusal enamel) and with wear (average thickness of 0.7 mm). (b) The crack initiation load and fracture load for the normal tooth and worn teeth.

Apart from existing controversies concerning causative risk factors and the difficulties in the diagnosis of cracks in teeth, the prevention and management of these cracks poses a greater challenge for practitioners. Currently, there is little agreement among clinicians

regarding the necessity, type and extent of the protective restorations for cracked teeth. Various procedures have been suggested for the management of a cracked tooth, including no treatment and observation, occlusal adjustment, sedative interim restorations, placement of orthodontic bands, interim crowns, direct or indirect composite resin restorations, complex and bonded amalgam restorations, and partial and complete indirect crowns [28]. However, none of the suggested approaches is yet considered as the standard of care for cracked teeth.

In the current study, we investigated the effect of a non-operative and conservative treatment with resin infiltration on the demineralized carious enamel through XFEM analysis. For the caries infiltration technique, a low viscous resin is applied on the demineralized enamel. The infiltrated resin penetrates into the lesion pores of enamel driven by capillary forces [339]. The simulation results of the fracture behavior of resin infiltrated lesion showed that following the application of resin on carious models, the crack initiation load and the fracture load values could recover significantly (up to 75% and 90% of the values for the corresponding sound tooth models respectively). Since many of the fissural caries and even small cracks at the base of the occlusal fissure remain undiagnosed even using conventional X-rays, the application of the resin infiltration technique can provide a safe and non-invasive option for the prevention of the formation and propagation of the cracks in demineralized fissural enamel. It is worth mentioning that the properties and the effect of the fissure seal materials which contain some amount of filler may be different from the no filler containing resin used for resin infiltration technique and therefore needs to be further investigated.

Considering the role of wear related factors in the formation and propagation of cracks in teeth, we should also emphasize the importance of preserving the integrity and anatomy of the proximal marginal ridge for minimizing cuspal flexure and maintaining the mechanical

strength of the tooth structure. Adjustment of the occlusal contacts in cases where a plunging cusp is in premature contact with the opposing marginal ridge, usually due to tooth rotation or overeruption, seems to prevent the attrition and deterioration of the marginal ridge anatomy. Also, in the case of proximal caries, the preservation of the marginal ridge using conservative methods such as tunnel preparation which preserves the integrity of the marginal ridge may provide greater mechanical advantage compared to conventional box preparation method. Treatment of the underlying conditions such as gastric reflux or bruxism to stop the gradual loss of enamel thickness should also be among the first treatment steps if observed in the patient.

In this study a series of caries and wear related risk factors at the tooth level were identified which can potentially increase the susceptibility of the tooth to fracture. These factors which include the large size of the pulp relative to the tooth volume, weakness or absence of proximal marginal ridge, less thickness of the enamel especially at the base of the occlusal fissure, steep occlusal cusp angle and the demineralization of the enamel at the base of the occlusal fissure should be considered and taken into account by clinicians along with the individual level risk factors such as bruxism and patient occlusion. The role of iatrogenic factors such as cavity design and restoration parameters in the initiation and propagation of teeth shall be the focus of future work.

4.5 Conclusion

This chapter explored the effect of occlusal wear and caries lesion on the mechanical performance and structural integrity of posterior teeth. Presence of fissural caries, worn proximal marginal ridge and decreased enamel thickness due to occlusal wear, imparted a

significant negative effect on the crack initiation load value of the lower molar models. Accordingly, models with intact and strong proximal marginal ridge, generally exhibited higher crack initiation loading, regardless of caries size and location. On the other hand, decreased cuspal slope due to occlusal wear and shrinkage of the pulp due to caries appeared to have a protective role and a direct relation with the fracture resistance of the tooth. Presence of fissural caries, if not treated (either with remineralization, resin infiltration or restoration), can be a major risk factor in the initiation of tooth fracture. The findings of this study emphasize the importance of early interventions in the management of caries for the prevention of future cuspal or tooth fracture especially in subjects with higher risk factors for tooth fracture such as caries, wear and bruxism.

Chapter 5: Effect of restorative materials and structures on monolithic dental crown fracture

Over the past decades, monolithic dental crowns have been widely used to restore cracked teeth or severe caries lesion. Ceramic crowns present numerous favourable characteristics including biocompatibility and excellent potential to simulate the optical characteristics of natural teeth. However, the evaluation of clinical survival rates of posterior all-ceramic crowns reveals the vulnerability to various failure mode. This study aimed to investigate the collective influence of material properties and design parameters on the fracture behavior of monolithic dental crowns. Comparing the critical load of crack initiation for different models with the maximum biting force revealed that for the studied monolithic materials, an optimum combination of design parameters in terms of tooth conservation and fracture resistance is determined. Among various CAD/CAM materials, zirconia crowns exhibited sufficient strength for a more conservative design with less thickness.

5.1 Introduction

Monolithic dental crowns fabricated via computer-aided design and manufacturing (CAD/CAM) technology have been widely employed in prosthetic dentistry in recent years attributable to their high level of dimensional accuracy, marginal adaptation and attractive optical characteristics [340-342]. In addition, they present lower risk of lab processing errors and cohesive failure compared with classically veneered frameworks [343, 344]. Despite

their many advantages, ceramic crowns are potentially susceptible to mechanical failure, possibly resulting in catastrophic fracture and chipping [345, 346].

Mechanical performance of ceramic materials is dominated by their compositional and microstructural properties as well as presence of defects and impurity phases. Accordingly, there has been continuous development of new CAD/CAM materials with enhanced mechanical properties through modification of composition and reduction of structural flaws. Currently, a variety of materials such as glass ceramics, zirconia, hybrid resin ceramics and polymer infiltrated ceramics are commercially available for constructing monolithic crowns in clinic [347]. The most recently developed hybrid materials benefit from the structural and property combination of high strength ceramics and more compliant polymers [348].

Among these hybrid materials are heavily particle filled ceramic resin nanocomposites, polymerized under high-temperature (180-200°C) and high-pressure (300 MPa) conditions in order to achieve a higher degree of conversion and polymerization as well as improved mechanical properties [349]. A novel type of hybrid material is Enamic, which is a polymer infiltrated ceramic network (PICN) material, developed through infiltration of a pre-sintered porous ceramic network (80% volume fraction) by the resin which fills the residual porosity of the ceramic and creates a dual network of ceramic and resin [348].

Not only do the clinical performance and durability of ceramic dental crowns depend on the physico-mechanical properties of the basic prosthetic materials, but are also determined by a range of clinical design parameters such as the thickness, preparation height, margin geometry, cusp inclination as well as the presence of surface irregularities and sharp features of the occlusal anatomy. Researchers have investigated different mechanical properties of

CAD/CAM crown materials and the effects of design and preparation factors on the fracture behavior of the monolithic ceramic crowns *in vitro* [144, 350, 351].

Considering the variations in experimental methods and fabrication of specimens, however, systematic experimental and numerical studies are still needed to understand the collective role of structural variables and material properties (elastic modulus and toughness) in this process. Therefore, the current paper provides a comparative study using three-dimensional (3D) extended finite element method (XFEM) to explore stress distribution, crack initiation and fracture pattern of five types of monolithic dental crown materials with various clinical design parameters. Analytical formulation, *in vitro* fracture tests and fractographic analysis of dedicated models were also performed to validate the findings of the simulation study.

5.2 Materials and methods

5.2.1 Micro-CT scanning and development of finite element models

An extracted human premolar tooth (Ethics protocol No X12–0065 & HREC/12/RPAH/106) was imaged using a high-resolution desktop micro computed tomography system (Skyscan 1172, Skyscan N.V, Aartselaar, Belgium) at an accelerating source voltage of 100 keV, a source current of 100 μ A, and an exposure time of 885 ms, resulting in an 8.9 μ m voxel size. The generated tomographic images were imported into ScanIP (Simpleware Pty. Ltd, UK) to segment the different anatomical parts of the tooth including enamel, dentine and pulp. Following surface refinement of the model components, the parameterized solid model was exported as an IGES file to SolidWorks (SolidWorks Corp., USA) to predominantly replace the enamel part of the tooth by a ceramic crown with a

shoulder margin. **Figure 5.1** illustrates the various design variables of the crown models. Three cusp angles (50°, 60°, 70°) and three different crown thicknesses (thin, medium and thick) at different parts of the crown, including buccal, lingual and occlusal area (**Table 5.1**), were adopted to construct different crown models.

Table 5.1: Thickness values at different parts of the crown for different groups (thin, medium and thick).

Thickness	Thin	Medium	Thick
Margin thickness (mm)	0.7	1	1.3
Occlusal and buccal-lingual thickness (mm)	1.05	1.5	1.95

The cusp angle was defined as the angle between the slope of the cusp (blue dashed line in Figure 5.1) and the vertical reference plane (red dashed line in Figure 5.1). Two designs, namely a rounded (U) and a sharp (V) design (**Figure 5.1(a)**), were considered here for the occlusal features of the crown. The cement component of the model was created by offsetting the upper dentine surface by 0.1mm [352] in SolidWorks (SolidWorks Corp., USA). The assembly of different components, including the restorative crown, dentine, pulp, adhesive cement and the loading ball, are shown in **Figure 5.1(b)**. During the assembly, the interfaces between the different components, including crown, cement and dentine, were assumed to be all bonded perfectly. The loading ball was carefully placed on the occlusal surface of the crown and was in frictional contact with both cusp slopes.

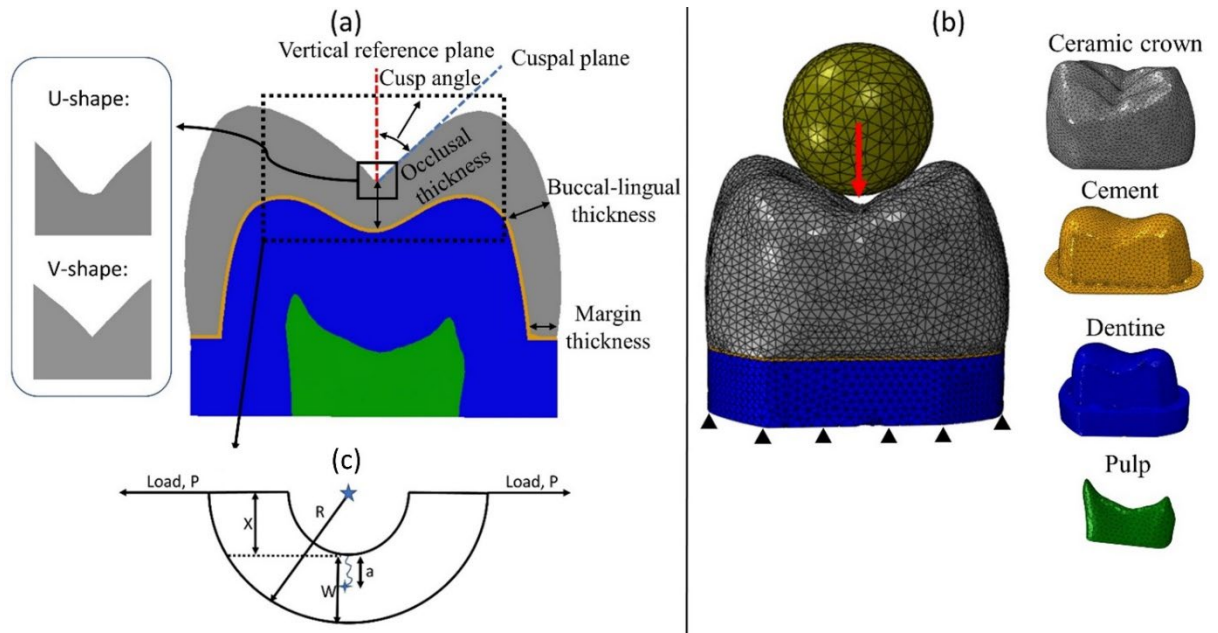


Figure 5.1: (a) 3D solid model of a premolar tooth with sharp (V shape) and rounded (U shape) occlusal anatomical features. (b) The assembled 3D finite element model consisting of the loading ball, ceramic crown, adhesive cement layer, dentine, and pulp. (c) C shape Compact-Tension (CT) model employed to simplify the crown geometry and derive the fracture load expression.

The finite element (FE) models were meshed using four-node linear tetrahedron elements. The mesh convergence test was conducted to determine the appropriate mesh size for the models by balancing the computational accuracy and cost [170, 285]. According to the convergence test, the global mesh size was 0.1 mm for the tooth/crown model and 0.8 mm for the loading ball; consequently, the corresponding number of elements was 259,294 (Degree of Freedom - DOF: 141,504) and 948 (DOF: 686), respectively.

The models were loaded using a 5 mm ball controlled by a downward force, linearly increasing from 0 to 10 kN. The loading ball was modeled to be a rigid body [103] and the contact between sphere, and crown surface was assigned a friction coefficient of 0.3 [105]. All the FE models were kinematically constrained on the bottom surfaces of the dentine and pulp [286, 287], as shown in **Figure 5.1(b)**.

5.2.2 Material properties of the components of the FE model

Five different types of the CAD/CAM materials were investigated in the study, namely (1) lithium disilicate (LDS) (e.g. Ivoclar, IPS e.max CAD), (2) feldspar ceramic (FC) (e.g. Vita, Mark II), (3) yttria stabilized tetragonal zirconia (Zr) (e.g., Ivoclar, E.max Zircad), (4) hybrid high-performance polymer (HPP) composite resin (e.g. GC Cerasmart), and (5) hybrid polymer-infiltrated ceramic (PIC) (Vita, Enamic). **Table 5.2** summarizes the material properties for each component in the FE models. All the materials were considered to be isotropic and homogeneous [105].

Table 5.2: Material properties of the components of the FE model, adopted from the literature [101, 274, 276, 292, 293].

Materials	Young's Modulus E (GPa)	Poisson's Ratio ν	Tensile Stress σ_{TS} (MPa)	Fracture Toughness K_{IC} (MPa·m ^{1/2})	Strain energy release rate G (J/m ²)
Lithium disilicate (LDS)	98	0.23	210	2.27	52.6
Yttria stabilized tetragonal zirconia (Zr)	204	0.27	865	5	122.5
Hybrid polymer-infiltrated ceramic network material (PIC)	35	0.23	148	1.2	41.1
Feldspar ceramic (FC)	72	0.22	112	1.25	21.7

Hybrid high-performance polymer composite resin (HPP)	10	0.3	216	1.2	145.2
Cement	8	0.3	-	-	-
Dentine	20	0.31	-	-	-
Pulp	0.01	0.49	-	-	-

The critical strain energy release rate G (J/m²) is a key material parameter related to the fracture toughness K_{IC} (MPa·m^{1/2}), indicating the strain energy required to propagate unit area of crack extension, which can be calculated as follows:

$$G = \frac{K_{IC}^2}{E} \quad (5.1)$$

where E is the Young's modulus and K_{IC} is the fracture toughness of the material.

5.2.3 Extended finite element method (XFEM)

In the present study, the XFEM fracture analysis was conducted to simulate the initiation and propagation of cracks in the monolithic dental crown using Abaqus 6.14 (ABAQUS, Inc, Providence, RI). The cracking criterion used in this study was the maximum principal stress in terms of,

$$f^e = \frac{\sigma_1^e}{(\sigma_{max}^0)} \quad (5.2)$$

where σ_{max}^0 refers to the allowable maximum stress (fracture strength) of the CAD/CAM materials, σ_1^e is the first principal stress in element (e), and f^e represents the stress ratio, which determines if cracking will initiate in the element. A crack was assumed to occur when the maximum principal stress exceeds the pre-defined tensile strength of the material. The subsequent crack growth was associated with the strain energy release rate [109]. The

cracking region was only considered in the ceramic crown part in the XFEM models [103]. Detailed background information about the mechanics of XFEM fracture analysis can be consulted in literature [302].

5.2.4 Crack surface area determination

Fracture simulation results were post-processed using an in-house developed program to determine the exposed area of a crack. Measuring this parameter at every timeframe of simulation provided a means for quantitative assessment and monitoring of crack evolution in the 3D crown models, which are outlined as follows. First, each element of the model was interrogated to determine the subset for which the Abaqus output STATUSXFEM is equal to one. In the XFEM analysis, STATUSXFEM defines the state of the crack in each model. Specifically, a value of 0 represents an undamaged element; a value between 0 and 1 indicates that the element is damaged but is still able to withstand some traction forces; and a value of 1 shows that there is full fracture failure in the element with no traction force remaining, which also corresponds to the occurrence of the crack in the model. Second, for the given mesh type, i.e. linear tetrahedral in this study, the nodal level-set quantity that defines the cracking surface was interpolated throughout the elements to locate the zero crossings. Elements bisected by the crack would have three or four such crossings. Third, the crack surface was obtained as the union of all the elemental zero crossings.

5.2.5 Fabrication of monolithic ceramic crowns and compression testing

An in-vitro experiment was dedicated to the tests of the monolithic crowns to validate the XFEM simulation results. The STL files of the crown models, created in SolidWorks (Dassault Systèmes SolidWorks Corp., USA), were used by a dental milling system to

fabricate PIC (Enamic) and Zr (Zircad) crowns. A 3D printing system was used to fabricate the die parts for supporting the crowns during the physical experiment using STL files of the die models generated in SolidWorks (Dassault Systèmes SolidWorks Corp., USA).

The fabricated crowns were cleaned and checked for any defects. The abutment dies were then etched with 37% phosphoric acid for 20 s, in order to produce the highest bond strengths to ceramic crowns. Finally, the crowns were cemented on the dies using a dual cure cement (Total C-ram, ITENA CLINICAL, France). The margins of each crown were light-cured (Satelec Mini L.E.D) for 20 s on each tooth surface. Eighteen pre-molar crowns bonded to the abutments were tested in a universal testing machine (Instron 5965; Instron, Canton, MA) using a 4 mm diameter steel cylindrical bar at a cross head speed of 1 mm/min until fracture took place. This approach for testing all-ceramic premolars was initially developed by Burke and Watts [353].

5.3 Results

The influence of material properties and selected design variables on the fracture characteristics of crown models including maximum principal stress, crack formation pattern, crack initiation load and crack surface area are presented in the following sections.

5.3.1 Maximum principal stress

Maximum principal stress (MPS) criterion postulates that the crack will initiate if the MPS in the crown exceeds the pre-defined value and the crack will grow in a direction perpendicular to the MPS to release the maximum strain energy [86]. During the simulation the MPS contours in the crown models were extracted at the same time point so that the corresponding load values were equal for all the models.

Three regions were the most commonly observed areas of stress concentration within the crowns (**Figure 5.2**), which included the occlusal notch, areas adjacent to the contact points between the loading ball and crown surface, as well as the intaglio (internal) surface of the crown specifically in the occlusal area. **Figure 5.2(a)** shows the MPS distributions of two representative crown models (50° cusp angle, medium crown thickness and similar material properties) with two different occlusal notch designs (rounded U-shape and sharp V-shape, respectively). Accordingly, at a normal load of 150 N on the ball, the rounded notch design presented a lower peak MPS (86.94MPa) compared to the model with a sharp notch (101.83MPa). Coronal and sagittal views of the stress contours indicated that the rounded notch design, had a more even stress distribution in the entire crown and a reduced stress concentration in the central occlusal notch (**Figure 5.2(a)**).

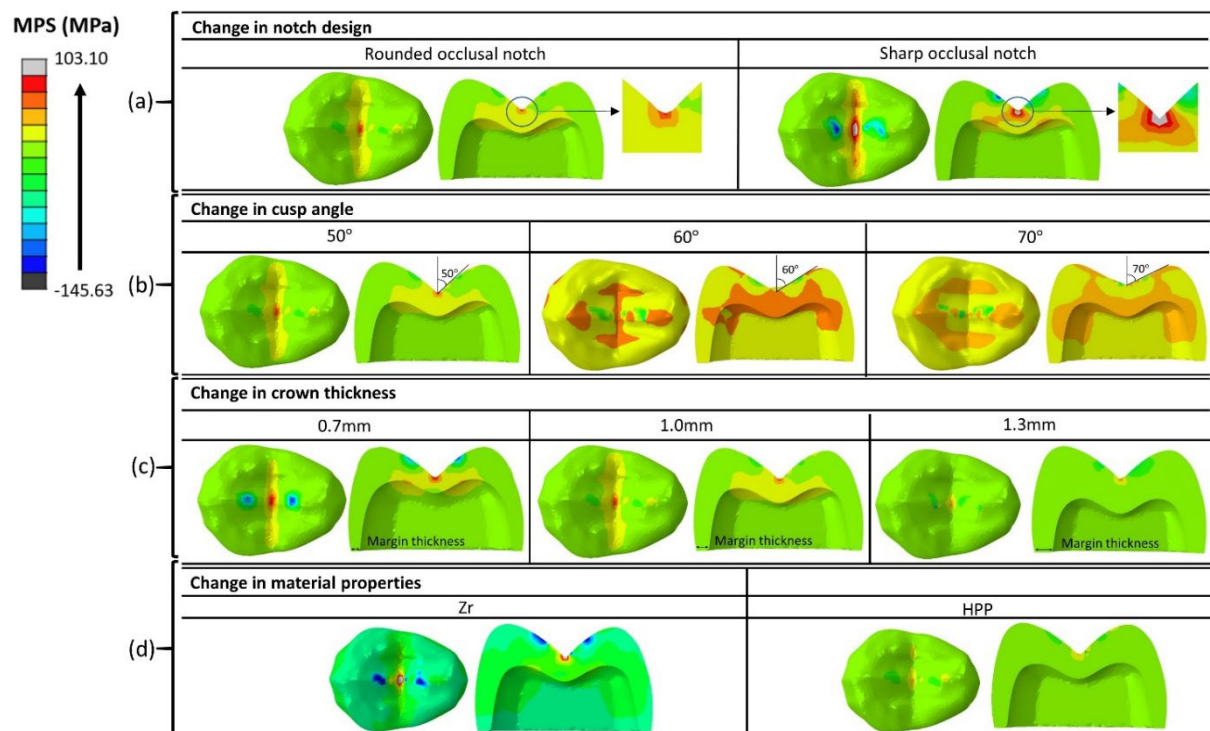


Figure 5.2: Coronal (top) and sagittal (bucco-lingual) views of the maximum principal stress (MPS) contours for the crown models under a load of 150 N, showing (a) the effect of

occlusal notch design (rounded or sharp), (b) the effect of different cusp angles (50°, 60°, and 70°), (c) the effect of various crown thicknesses (thin, medium and thick), and (d) the effect of material properties (Zr with $E = 204$ GPa and HPP with $E = 9.92$ GPa).

Figure 5.2(b) depicts the principal stress distributions for three crown designs with the same thickness (medium), notch design (rounded) and material properties but different cusp angles, i.e. 50°, 60° and 70°. It was found that the model with 50° cusp angle had the highest peak MPS value (17.75MPa), followed by the models with 60° (15.96MPa) and 70° (8.98 MPa) cusp angles under the same loading.

Not only did changing the cusp angle affect the magnitude of MPS, but also altered the distribution pattern of MPS in the crowns as shown in **Figure 5.2(b)**. While with a cusp angle of 50° (steeper cusps), MPS was mainly concentrated in the central groove area; the increase of the cusp angle to 60° (decreasing the steepness) resulted in a wider distribution of the MPS and its extension to the secondary occlusal grooves. Further increase in the cusp angle to 70° led to a more evenly distributed stress pattern, which almost eliminated the stress concentration from the central groove (**Figure 5.2(b)**).

Figure 5.2(c) shows the effects of crown thickness (thin, medium and thick) on the MPS magnitude and distribution pattern of the three representative crown models with a rounded notch, 50° cusp angle and the same material properties. In general, a greater thickness decreased the MPS value and generated smaller stress concentration areas in the crown. In the thick crowns, there was a shallow stress concentration area close to the occlusal notch surface; while in the thin crowns, the stress concentration area had a higher magnitude and extended to the internal surface of the crown.

Figure 5.2(d) shows the maximum principal stress (MPS) contours for the two nominated crown models with the same design parameters (50° cusp angle, rounded notch and medium thickness) but different material properties (HPP with a Young's Modulus of 9.92 GPa and a toughness of 1.2 MPa·m^{1/2}; and Zr with a Young's Modulus of 204 GPa and a toughness of 5 MPa·m^{1/2}). While the peak MPS for the crown was strongly affected by the material type, the stress distribution pattern was not noticeably different among various groups of materials. Accordingly, the peak MPS value at 130 N load exhibited an increasing rank for HPP (8.73 MPa), PIC (15 MPa), FC (16.95 MPa), LDS (17.75 MPa), and Zr (21.05 MPa) respectively, with central groove being the main stress concentration area in all these material groups (**Figure 5.2(d)**).

5.3.2 Crack initiation load

Figure 5.3 shows the crack initiation loads for the models made of the same material but with various cusp angles, notch designs and thicknesses. It was observed that in general, the crack initiation load rises with the increase in the cusp angle for different crown designs and material types. In most of the models, the increase in crack initiation load was more significant when the cusp angle increased from 50° to 60° compared to the increase from 60° to 70°. The effect of increasing cusp angle was less prominent in the thin crowns, in which a higher cusp angle did not enhance the fracture resistance of the crown.

Concerning the effect of occlusal notch design, the rounded notch geometry led to a higher load of crack initiation compared to the sharp notch for all the study materials. This effect was minimal in the thin crowns but more significant in the thick crowns, in which the crack initiation load almost doubled in the rounded compared to the sharp notch design.

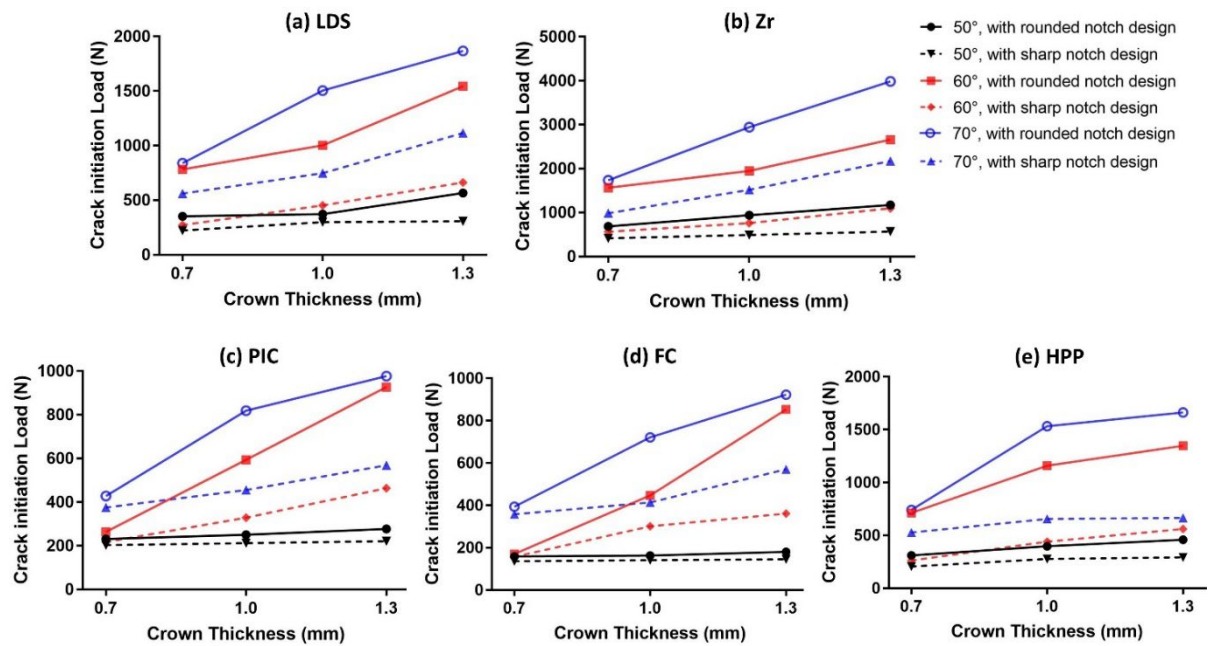


Figure 5.3: The crack initiation loads for different crown models made from five types of CAD/CAM materials namely (a) LDS, (b) Zr, (c) PIC, (d) FC and (e) HPP. Each figure shows the crack initiation load values for different crown designs with various cusp angles, notch designs and crown thicknesses.

Crown thickness was a key determinant of the fracture resistance in all the materials, and it had a direct relationship with the crack initiation load. Accordingly, a greater crown thickness resulted in a higher load of crack initiation in different models. However, the effect of cusp angle was dominant when the angle was in the low range of 50° for which increasing the thickness did not enhance the fracture initiation load.

In addition to various design parameters, material properties also had a significant effect on the crack initiation loads and fracture resistance of the crowns (**Figure 5.3**). Accordingly, the zirconia (Zr) crown models had the highest crack initiation load, followed by the LDS glass ceramic, HPP, PIC and feldspathic material (FC), respectively.

5.3.3 Crack surface area

The evolution of the crack surface area with increasing load for nominated crown designs and materials are presented in **Figure 5.4**. For different crown designs and materials, the crown models with the least thickness demonstrated increased crack surface area at the lowest load value compared to the medium and high thickness models (**Figure 5.4(a)**). The increased crack area at a lower load value was also observed for the crown models with sharp occlusal notch geometry compared to the rounded notch design (**Figure 5.4(b)**).

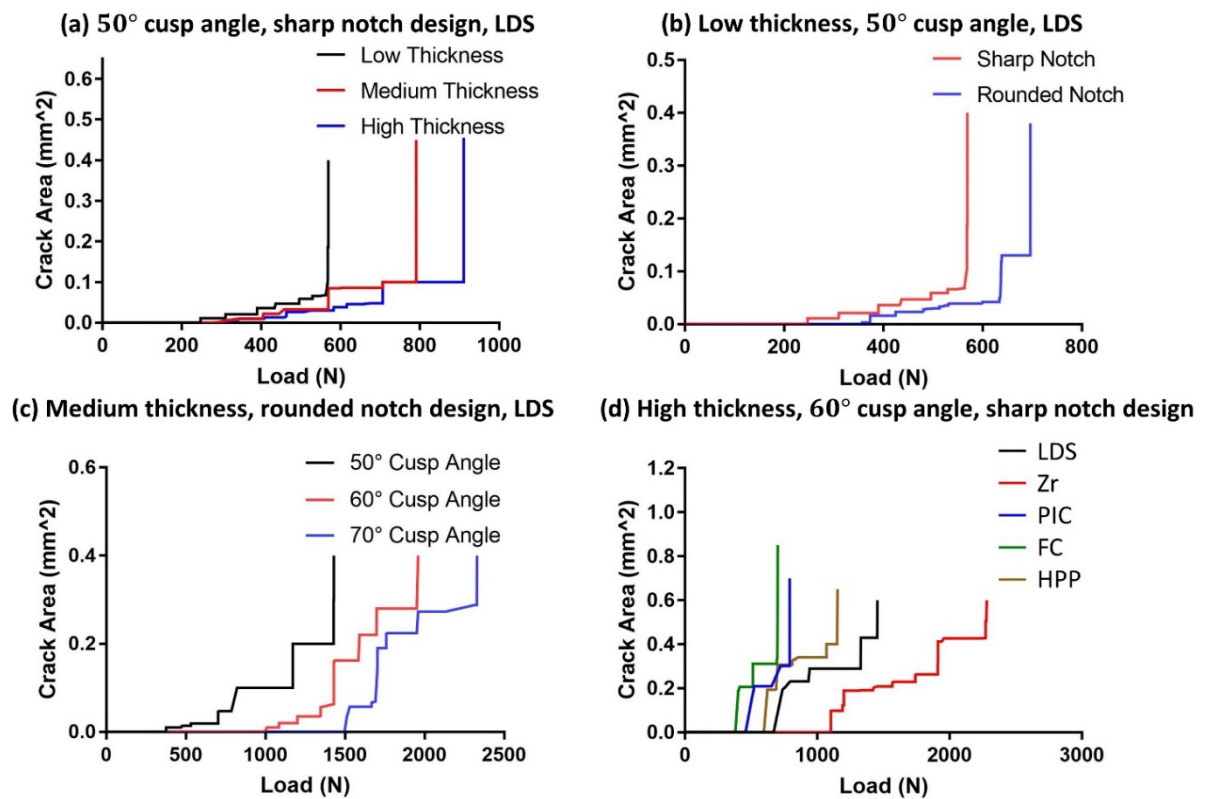


Figure 5.4: Evolution of cracked surface area with increasing load showing the effect of (a) crown thickness, (b) occlusal notch design, (c) cusp angle, and (d) material type for nominated crown models.

For the effect of cusp angle, a more acute angle led to a lower load at crack initiation, and a generally greater crack area for a given load. For instance, at a load value of 1400N, the model with 50° cusp angle already had catastrophic fracture with a crack area of 0.4mm², the crack surface area for the 60° cusp angle was under 0.2mm² then; whilst there was no crack in the model with 70° cusp angle yet (**Figure 5.4(c)**).

Regarding the effect of material type, FC was found to initiate cracking at the lowest load, followed by PIC, HPP, LDS and Zr, respectively. FC was the most brittle in the simulations, demonstrating a large increase in the crack surface area when there was a relatively small increase in the applied load (**Figure 5.4(d)**).

5.3.4 Crack pattern

The crack growth in all the investigated models was found to be stable, in which the crack was initiated at a lower load then progressively extended with increasing load until final fracture of the crown. The crack pattern and location for a representative model (PIC, rounded occlusal notch, medium crown thickness and 60° cusp angle) at different time points during the simulation (crack initiation, and propagation) are presented in **Figure 5.5**. In most of the crown models, the crack originated on the occlusal surface from the base of the occlusal notch where the stress concentration was the highest (**Figure 5.5(a)**). It then propagated along the length of the primary groove until it reached the proximal margins (**Figure 5.5(b)**), after which it grew in a downward direction and extended through the entire thickness of the crown (**Figure 5.5(c)**). According to the simulation results, the location of the crack was not affected by changing the crown thickness, notch design and material properties. However, for some very resistive crown models, e.g. with a high cusp angle,

greatest thickness and rounded occlusal notch, the crack initiation and extension occurred in the fissural area but at a point closer to the loading point (**Figure 5.5**).

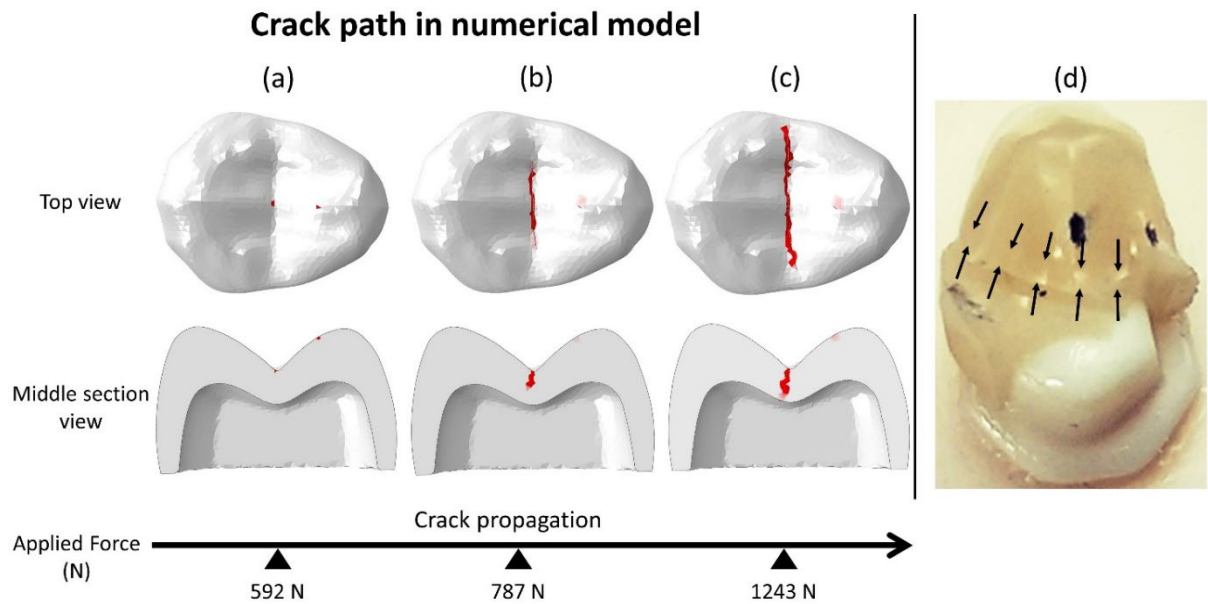


Figure 5.5: The simulated crack pattern and location at different time points for a representative model (PIC with rounded occlusal notch, medium crown thickness and 60° cusp angle), which shows (a) the initiation of the crack at the central groove, (b) the growth of the crack along with the central groove, (c) up to the marginal ridge, (d) the crack path in the tested physical specimen.

Examination of the fracture surfaces of the in-vitro tested crowns with scanning electron microscope (SEM) revealed multiple hackle lines, crack propagations and arrest lines in the fractured specimens. Fracture origins were identified in the fissure region as well as below the loading contact area at the occlusal surface of the crown with associated radiating hackle lines converging on this point (**Figure 5.6**). Multiple arrest lines were observed especially in fractured hybrid ceramic crowns, indicating higher fracture compliance compared to the zirconia crowns.

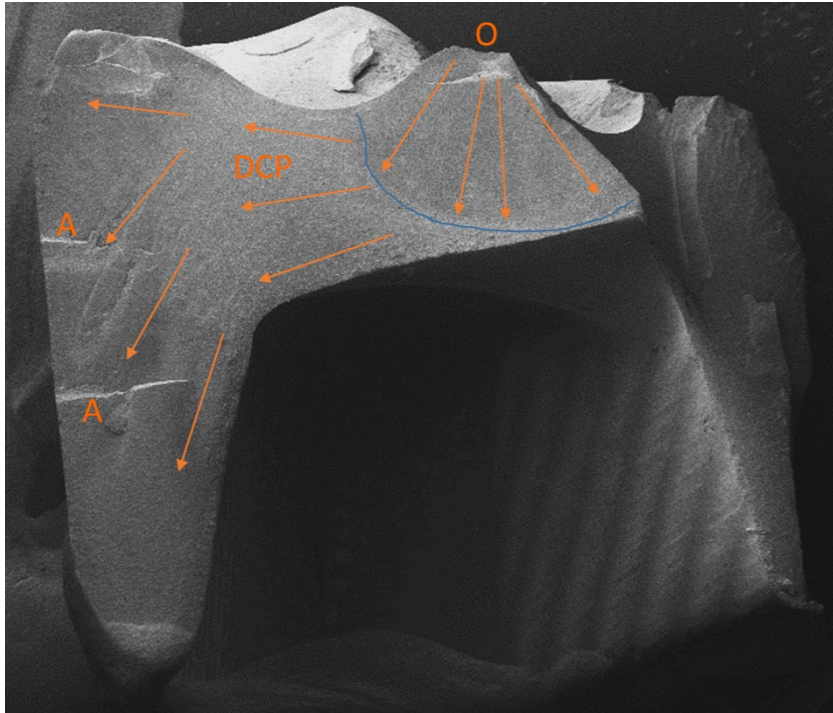


Figure 5.6: Scanning electron microscopy image of fracture surfaces of a fractured IPN showing a contact induced pop-in semi-circular crack. The arrows indicate the direction of the crack propagation (DCP) front moving along the arrowed path and reaching multiple arrest lines (A).

5.3.5 Experimental validations of the XFEM results

Figure 5.7(a) compares the force-displacement curves of the numerical (red line) and experimental (blue line) studies; and **Figure 5.7(b)** compares the fracture load values among experimental, numerical and analytical results for a nominated crown model (PIC, medium thickness, 60° cusp angle and rounded notch design).

In the experimental force-displacement curve (in blue), the first major drop in the force was recorded at the crack initiation stage. At the final stage of the experiment, the loading force dropped suddenly when it reached the ultimate strength of the crown structure, in which

the sample experienced complete bulk failure. According to the simulation results, the premolar crown model exhibited almost linear force-displacement behaviour with a few small load drops and a large drop prior to the catastrophic failure. This drop resulted from the loss of stiffness in certain elements due to crack initiation. Comparing the XFEM simulation with the experimental test, good correlation can be identified in the fracture patterns, in which both the experimental and simulated cracks initiated from the bottom of the central occlusal fissure, and then propagated towards the proximal margins and proximal surfaces of the crown.

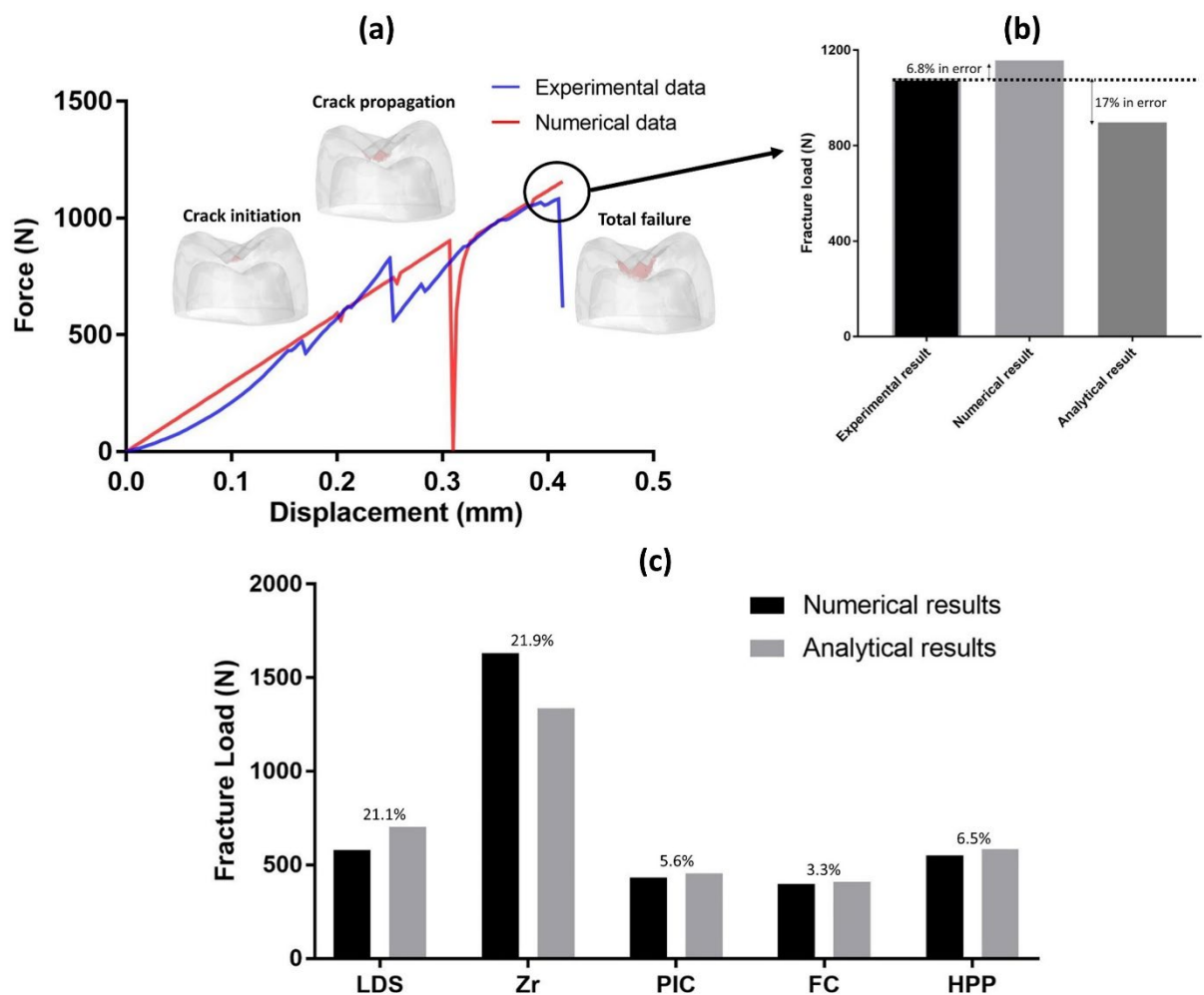


Figure 5.7: (a) Force - displacement curve generated from the numerical (red line) and experimental (blue line) data for a nominated crown model (PIC, medium thickness, 60 °

cuspal angle and rounded notch design) showing the load values for the crack initiation and total failure of the crown; (b) Comparative fracture load values among experimental, numerical and analytical results for the nominated crown; (c) Fracture loads from analytical and XFEM numerical data for a nominated crown model (low thickness, 50 ° cuspal angle and sharp notch design) exhibiting a reasonable agreement between the two methods for various crown materials.

The simulated crack initiation load and total failure load also exhibited reasonable agreement with the experimental results. It should be noted that since a loading ball was used for the simulation part of the study, the authors initially tried using a steel ball for the laboratory experiment as well. However, lack of stability of the ball on the premolar cuspal slopes, led to the selection of a cylinder for the experiment. Further validation of the simulation results was performed to estimate the effect of the difference in the loading element; and it was found that the XFEM results were very similar in terms of the crack initiation load (<6%) and final failure load (<8%) for the same model loaded with either a ball or cylinder (Appendix 1). Likewise, the fracture path was also almost identical for these two cases.

5.4 Discussion

Computational methods have compelling benefits for the fracture study of brittle materials with complicated geometry, such as dental crowns. This is because the issues caused by asymmetry and misalignment of specimens in experimental settings cannot be compensated by small amounts of plastic deformation as happens for ductile materials; therefore potentially causing uncontrolled fracture behaviour and associated scatter of testing results in such experiments [354]. In the present study, an *in-silico* computational modelling

approach called eXtended Finite Element Method (XFEM) was adopted here as it has been shown to have high predictive ability in forecasting the fracture behaviour of complex structures. A key advantage of XFEM for fracture studies is its independence of the element mesh from the morphology of the crack surface and crack front [355]. This eliminates the need for remeshing during crack propagation and therefore enables convenient simulation of crack evolution.

The developed XFEM model for quantifying the crack surface area also provided an accurate approach for observing the evolution of the crack through different stages including crack initiation, stable propagation and final catastrophic failure. For some of the cases, the crack surface area showed a steady or gradual growth following crack initiation (see **Figure 5.4**), indicating the fracture resistance of the structure to the localized ball loading condition and restriction of the crack propagation. With increasing loading, there was usually a significant final jump in crack extension in most of the models (**Figure 5.4**), which indicates catastrophic propagation of crack; and the corresponding load values were deemed the fracture load. The simulated fracture load obtained from the quantification of XFEM crack surface area also showed strong correlation with that obtained from the experimental testing of the crowns.

As shown in **Figure 5.2**, stress concentration was more evident in three regions within the crowns, which were the occlusal notch, areas adjacent to the loading contact points, as well as the intaglio surface of the crown particularly in the occlusal area. The locations of these stress concentration areas identified in the simulation (**Figure 5.2**) well correlate with the common areas where different types of cracks develop in structurally failed crowns [356]. Accordingly, while splitting cracks mainly initiate in the central occlusal fissure, it is

observed that contact-driven Hertzian cracking can develop beneath the contact points with the loading body (opposing tooth or the indenter). Tensile stresses at the internal surface of the crown generated from the flexure of the crowns under occlusal loading also cause flexural radial cracking, starting at the crown internal surface and growing towards the occlusal surface or the margins of the crown [356]. Although the competitive distribution and magnitudes of stresses among these regions depends on the geometrical parameters of the crowns, the observed fracture mode in our study was predominantly the splitting bulk fracture (Mode I). The crown material properties would mostly have an effect on the magnitude, but not on the distribution pattern of the MPS among the different models simulated.

In addition to the thickness, cusp angle and notch design, two other interesting anatomical features were also found to play a key role in increasing the fracture resistance of the crown models. First, proximal marginal ridge at the two sides of the crown demonstrated a reinforcing and resistive role against splitting of the crown through confining the propagation of the splitting crack (**Figure 5.5(c)**). In general, propagation of the crack along the primary groove arrested when it reached the marginal ridge, where it changed direction and grew downward. Apparently, lack or weakness of proximal ridge may be a potential factor in facilitating the splitting fracture of the crown. This highlights the importance of optimum design for the thickness and height of the marginal ridge area in restorative crowns considering that the marginal ridge is also the location of contact with the opposing cusp tips in the posterior teeth. Second, occlusal fissures also contributed to distributing and directing the stress away from the primary groove and towards the buccal and lingual cusps of the crown, therefore diminishing the stress concentration in the central primary groove (**Figure 5.2**).

Regarding the effect of occlusal notch geometry on the fracture resistance of the crown, the XFEM results confirmed that the presence of a sharp occlusal notch caused a higher stress concentration and significantly lower crack initiation load for all the materials, crown thicknesses and cusp angles considered in this study. As shown in the previous *in-vitro* experiments [305, 357], a rounded and curved notch morphology allows the stress to distribute more evenly and over a wider surface area, thereby preventing the concentration of the stress in the notch area.

Any surface irregularity including the sharp occlusal notch can be considered as a discontinuity in the microstructure of the material which can predispose the crown to crack initiation. This highlights the need for careful consideration by technicians and clinicians during the design, fabrication and occlusal adjustment of the crowns to avoid the generation of any surface irregularities or sharp points [358].

The cusp angle also played a significant role in the fracture resistance of the crowns, which affected the MPS distribution, crack initiation load and crack surface area to different extents in the different models. Similar to the findings in the previous laboratory experiments [305, 357], increasing the cusp angle resulted in higher fracture resistance of the crown presumably through the reduction of the lateral force component of the applied load and the resultant tensile stress around the occlusal notch area. A low cusp angle of 50° (steeper cusp) led to a significant reduction in the crack initiation load and a more localized MPS distribution in the crowns. The effect of a low cusp angle was dominant and generally, it could not be compensated by changing the material type and/or increasing the crown thickness.

By comparing the average maximum bite force (800 N in the posterior region [359]) and the crack initiation load from each model, we could detect the safe cusp angle for a specific combination of material type and crown thickness. Accordingly, a steep cusp angle of 50°, resulted in a crack initiation load lower than the maximum bite force (800 N) for all the materials and thicknesses, except for medium to high thickness zirconia crowns with a rounded notch design that had a crack initiation loads of 939 N and 1174 N, respectively.

At a cusp angle of 60°, merely the crown designs with high thickness and rounded notch were within the safe range of the load values for FC (853 N) and PIC (927 N). However, with increased material toughness in HPP, LDS and ZR, the medium thickness designs also achieved a higher crack initiation load than the maximum bite force of 800 N. While increasing the cusp angle from 60° to 70° in the medium thickness designs could bring the crack initiation load of FC and PIC crowns close to the maximum bite force, it was still below the maximum bite force (394 N for FC and 428 N for PIC) for their low thickness designs. These findings confirm the idea that a safe cusp angle could become steeper when the fracture toughness of the crown material increases [305].

Crown thickness is a key clinical parameter during the preparation of the full coverage restorations; and clinicians commonly aim to achieve the most conservative yet strong design for the crowns. This issue is of more importance to the posterior crowns where higher occlusal forces and loading contacts are typically imposed on the teeth. In the current study, the thickness displayed a considerable effect on the fracture resistance of crowns, with a higher thickness resulting in decreased stress concentration and a more even distribution of the MPS in the crowns (**Figure 5.2(c)**). The thickness of the crown also revealed a direct relationship with the crack initiation load in most of the models except for the models with

low cusp angle (50°), where there was no significant difference among the crowns with different thicknesses (**Figure 5.3**).

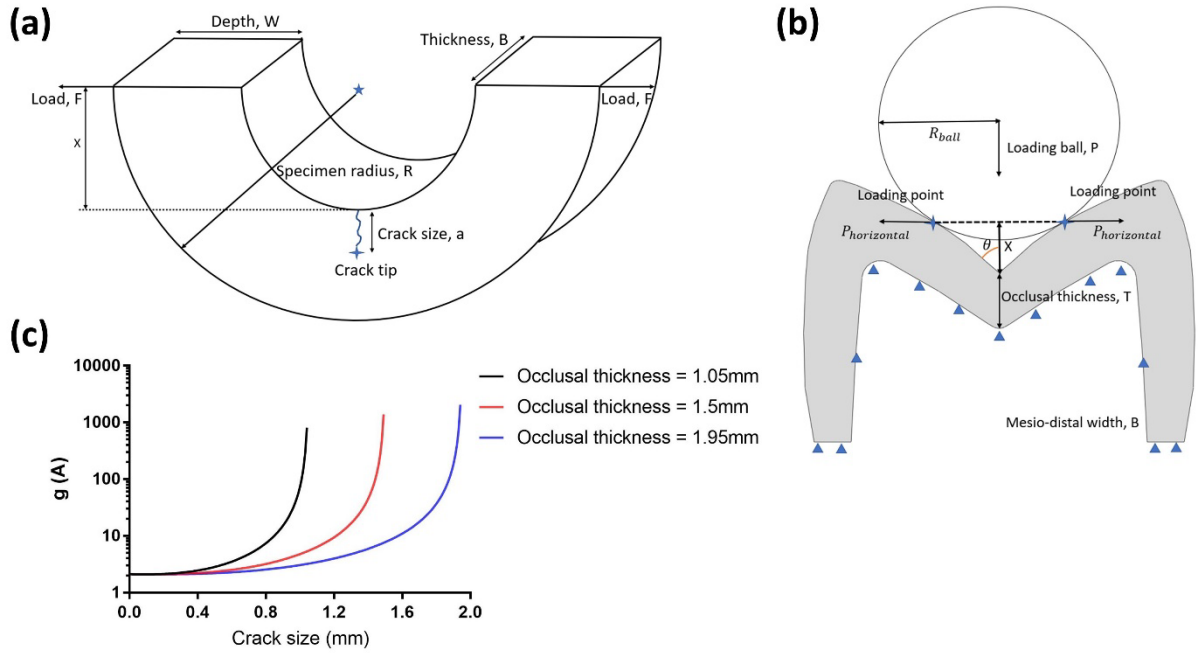


Figure 5.8: (a) Standard C shape Compact Tension (CT) model, ASTM E-399 Standard Specimens. (b) Buccal-lingual sectional view of crown and loading ball. (c) Plot of crack size function $g(A)$. Note that there is a plateau at $g^*=2.1$, indicating a relative stable period before the stress intensity factor rises and crack becomes unstable.

The relation between failure load and design variables, including notch design, cusp angle (θ) and crown thickness (T), can be considered in terms of the stress intensity factor (K_I). As the geometry of monolithic crown is rather complex, it is challenging to estimate the stress intensity factor directly. According to the studies by Barani et al [13] and Sornsuwan

and Swain [305], the splitting configuration might be likened to the mode I compact tension (CT), which assumes the notch as a crack. The expression of stress intensity factor for standard C-shape CT model, shown in **Figure 5.1(a)** and **Figure 5.8(a)** can be written as [360, 361],

$$K_I = \frac{F}{WB} \sqrt{\pi a} \cdot Y_{CT} \left(\frac{W}{R}, \frac{X}{W}, A \right) \cdot g(A) \quad (5.3)$$

where F is the applied force, W is the specimen depth, B is thickness, a is a crack size, R is specimen radius, X is the moment arm of the crack origin, A is relative depth of the crack, defined by $A = a/W$, Y_{CT} is geometrical factor, and $g(A)$ a dimensionless crack size function.

As illustrated in **Figure 5.8(a)**, where F is applied load, W is specimen depth, B is thickness, R is specimen radius, X is the distance from loading point to the crack origin. In addition, Y_{CT} is a geometrical factor and $g(A)$ is a crack size function, which can be written as,

$$Y_{CT} \left(\frac{W}{R}, \frac{X}{W}, A \right) = \left(3 \frac{X}{W} + 1.9 + 1.1A \right) \left[1 + 0.25(1 - A^2) \frac{W}{R} \right] \quad (5.4)$$

$$g(A) = \frac{3.74 - 6.3A + 6.32A^2 - 2.43A^3}{\sqrt{\pi}(1-A)^{3/2}} \quad (5.5)$$

where A is the relative depth of the crack, shown as $A = \frac{a}{W}$.

By comparing the C-shape CT model with the geometrical features of a monolithic crown in the buccal-lingual sectional view (**Figure 5.2(b)**), the above parameters can be presented by,

$$W = T \quad (5.6)$$

$$R = R_{ball} + T \quad (5.7)$$

$$X = R_{ball} \frac{\cos^2 \theta}{\sin \theta} \quad (5.8)$$

where T is the occlusal thickness, R_{ball} is the radius of the loading ball, which is a constant (2.5mm here).

Upon introducing the applied load (P), cusp angle (θ), and occlusal thickness (T), the expression of stress intensity factor K_I can be written as:

$$K_I = \frac{P_{horizontal}}{TB} \sqrt{\pi a} \cdot Y_{CT}(T, \theta, A) \cdot g(A) \quad (5.9)$$

where A is the relative depth of the crack compared to the occlusal thickness, shown as $A = \frac{a}{T}$,

and $P_{horizontal} = \frac{P}{2 \tan \theta}$.

Then by integrating the geometrical features of monolithic crown into the C-shape CT model, Y_{CT} can be expressed as:

$$Y_{CT}(T, \theta, A) = Y_{CT}(T, \theta) = \left(C_1 \frac{T}{5+T} + C_2 \right) \left[C_3 \frac{\cos^2(\theta)}{T \sin \theta} + C_4 \right] \quad (5.10)$$

According to the curve fitting using the data from finite element analysis, the values of constant C_1, C_2, C_3, C_4 can be obtained, resulting in specific Y_{CT} as:

$$Y_{CT}(\theta, T) = -36.2 \frac{R \cos^2 \theta}{(R+T) \sin \theta} + 39.4 \frac{T}{R+T} + 5.9 \frac{R \cos^2 \theta}{T \sin \theta} - 0.2 \quad (5.11)$$

Regarding the crack size function ($g(A)$), the plot (**Figure 5.8(c)**) shows that $g(A)$ remains at a plateau level of $g^*=2.1$, followed by a drastic increase, suggesting that the crack

will propagate steadily until reaching a critical relative depth of the crack (when $A = a/T = 0.75$), at which point the final instability occurs and the model splits. In order to simplify the expression of fracture load, it can be assumed that the fracture occurred when the relative depth ($A = a/T$) attained a critical value of 0.75. Therefore, the crack size function can be treated as a constant, given by $g(A) = g^* = 2.1$, at $a_{critical} = 0.75T$.

In order to incorporate the effect of Young's modulus in the equation, the normalized Young's modulus of crown materials, E_0 , can be used,

$$E_0 = \frac{E_{crown}}{E_{dentine}} \quad (5.12)$$

where E_{crown} is the Young's modulus of crown, and $E_{dentine}$ is the Young's modulus of dentine.

When $K_I = K_{Ic}$, the critical fracture load $P_{critical}$ can be derived, with a broadened scope for all material types by further including normalized Young's modulus, E_0 , as,

$$P_{critical} = \frac{\eta \tan \theta K_{Ic} T^{1/2} B}{E_0^{0.2}} Y_{CT}(\theta, T)^{-1} \quad (5.13)$$

where η is a dimensionless constant, 0.24, and K_{Ic} is fracture toughness ($MPa \cdot m^{1/2}$), T is occlusal thickness (mm), B is mesiodistal width (assumed as a constant with 6mm in this study), θ is cusp angle ($degree$), Y_{CT} is dimensionless crown geometry factor, and the unit of force is kN .

The XFEM data exhibits a reasonable agreement with the above critical load expression (with a regression of R^2 value of 0.82) (**Figure 5.7(b)** and (c)). Note that while the force expression (Eq. (5.6)) does not include the uncertainties of a 3D monolithic crown, it exhibits

the role of crown geometrical parameters, which provides a useful relationship to estimate the fracture load.

While for different materials, only medium and high thickness models presented a crack initiation load above the maximum bite force (800N) for both 60° and 70° cusp angle designs, zirconia had a crack initiation load value higher than maximum bite force even for its low thickness design as well (**Figure 5.3**). These results corroborate the previous studies that reported a direct relationship between the thickness and fracture load of monolithic crowns, and suggested a thickness value of 1.2 mm for lithium disilicate [362] and 1 mm for Zirconia crowns [363]. Regarding the effect of thickness on the fracture resistance of the crowns, it is suggested that the load required for bulk fracture in ceramic restorations is proportional to the square of the ceramic thickness [364-366]. The reduced crack initiation load in low thickness crowns can be attributed to the increased flexural and tensile stress on the intaglio surface of the crown (**Figure 5.2(c)**) which can potentiate the crack initiation.

Within the limitations of the present study, it can be concluded that the critical loads for crack initiation in monolithic crowns can be associated with material properties and design parameters such as the thickness, cusp angle and occlusal notch design. Accordingly, a design with a rounded notch, 70 ° cusp angle and medium thickness (1.5 mm occlusal) seems to be an optimum combination of design parameters in terms of tooth conservation and failure resistance for different types of monolithic materials including FC, PIC, HPP and LDS. Zr seems to possess sufficient strength for a lower thickness (0.7 mm marginal and 1.05 mm occlusal) as well as a lower cusp angle (60 °). Considering the improved esthetics of high translucent zirconia ceramics but their lower fracture toughness (4 and 3 MPa.m^{1/2} for 4 and 5 mol% yttria zirconia), the expression in Eq. (5.6) suggests that these crowns would have a

proportionally lower resistance to splitting fracture compared with the higher toughness of the 3 mol% yttria zirconia. It should be noted that since the bite force is typically distributed among several teeth in normal functional conditions, the maximum bite force for each single tooth contact would be lower than the overall value. However, in this study the worst-case scenario was considered regarding the maximum bite force to evaluate the reliability of the monolithic crowns in extreme situations such as parafunctional or singular heavy contacts. In the current study, due diligence was exercised to simulate the conditions of laboratory load-to-failure tests, however similar to any other numerical work, the results should be interpreted with further caution. In addition, while the focus of the current study was on the crown thickness, cusp angle, notch design and material type of the crown, other factors such as the margin design, cement properties, crown height and wall taper also influence the fracture behavior of the crowns, which can be a topic of future research.

5.5 Conclusion

In this chapter, three-dimensional (3D) models with different combinations of design parameters (thickness, cusp angle and occlusal notch geometry) and material type (lithium disilicate, feldspar ceramic, zirconia, hybrid resin ceramic and hybrid polymer-infiltrated ceramic) were developed for the failure analysis using XFEM to identify the stress distribution, crack initiation load, fracture surface area and fracture pattern. In-vitro fracture tests and fractographic analysis of dedicated models were also performed to validate the findings of the XFEM simulation. Based on the simulation results, a mathematical formula was proposed to express the relationship between the fracture load and the geometrical factors of crowns. Comparing the critical load of crack initiation for different models with the maximum biting force revealed that for the studied monolithic materials excluding zirconia, a

design with a rounded occlusal notch, 70° cusp angle and medium thickness (1.5 mm occlusal) is an optimum combination of design parameters in terms of tooth conservation and fracture resistance. Zirconia crowns exhibited sufficient strength for a more conservative design with less thickness (1.05 mm occlusal) and sharper cusp angle (60 °).

Chapter 6: On fatigue failure prediction of prosthetic devices through XFEM analysis

In addition to the dental restorations, orthopaedic prosthetic devices have been extensively used to treat a wide range of bone diseases and injuries. However, failure of these devices due to fatigue under cyclic loading has been recognized as a primary concern on therapeutic longevity. Experimental testing has long been a dominant approach to characterizing the fatigue behaviour of prosthetic devices. However, experimental methods could be of multiple shortcomings such as their restrictive nature *in-vivo* in medical studies and limitations of extrapolating the testing results. This study develops a numerical approach for modelling fatigue failure in some commonly-used osteofixation devices that are implanted to support various major bone defects/trauma and fractures. The eXtended Finite Element Method (XFEM) is employed herein to model fatigue crack formation and propagation as per level set functions to suppress the need for re-meshing. For validation purpose, a benchmark problem involving a modified compact tension structure is first carried out, in which the modelling results are compared with the relevant experimental data to demonstrate the effectiveness of the proposed XFEM approach. Further, two representative orthopaedic examples are studied for characterizing the fatigue behaviour of a femoral

osteofixation plate and a mandibular reconstruction mini-plate, respectively. The results reveal that healing/remodelling of grafted bone as well as tissue ingrowth to the scaffold have significant bearing on fatigue life of fixation plates. This study showcases a valuable approach for predicting fatigue failure of prosthetic devices *in-silico*, thereby providing an effective tool for design optimization of patient-specific prosthetic devices to ensure their longevity.

6.1 Introduction

Bone loss and defects caused by trauma, tumour or osteoradionecrosis have increased drastically over the past few decades. Applications of osteofixation/osteosynthesis devices, such as fixation plates, are considered fundamental to stabilize various treatments of bone defects for promoting osteointegration and reconstruction [367-369]. Not only does a fixation plate connect the individual bone segments and/or enable bone substitute to join the surrounding tissues, but also partially supports physiological loadings induced by daily movement, thereby maintaining system stability in the course of bone healing and regeneration [370]. In this context, a range of different fixation devices made of metallic alloys or other synthetic biocompatible materials have been widely used clinically. Nowadays the success rate of fixation systems has been enhanced through developing more appropriate biocompatible materials and fixation structures [371].

Despite extensive applications of various fixation prostheses, there are increasing case reports on the complications associated with such surgical strategy, in which screw loosening, plate exposure, and screw or plate fracture are some typical examples [372, 373]. Clinical observations and specialized literature have revealed that metallic fixation devices are often

subject to high stress, leading to fracture either by catastrophic overloading or cyclic fatigue failure [374]. Medical statistics show that plate fractures occur in 2.9–10.7% of treated cases [375, 376]. The failure of fixation plates may lead to severe clinical incidents and undesirable consequences by causing further damage to the supported bone and surrounding tissues, thereby resulting in additional injury and excessive cost to both patients and healthcare system [377]. Therefore, characterization and assessment of these failures in a predictive manner signifies a critical research issue. Although some clinical studies have reported that failure of fixation system occurs when the mechanical stresses within the plates exceed the ultimate strength of its materials [374, 375], more recent studies suggested that low-cycle fatigue may be a more common failure mode for the plates made of conventional stainless steel as well as some relatively newer metallic materials (such as titanium alloys), in which the mechanical stresses could be considerably lower than the ultimate strength of the plate materials [378].

To investigate the fatigue characteristics, physical tests are commonly carried out in practice [379, 380]. Nevertheless, such experimental methods are often too computationally expensive and/or too time-consuming, and sometimes difficult to capture important mechanics details, such as complex stress states during the crack propagation. Therefore, more efficient alternatives such as computational modelling approaches are drawing growing attention in fatigue analysis of engineering products [381]. For this purpose, the conventional finite element method (FEM) has been widely employed to scrutinize the fatigue failure of engineering structures mainly based upon conventional S-N curves of materials [382, 383], in which the stress distribution in the structures is first characterized and then compared against the S-N data obtained from standard material fatigue tests. The susceptible region of fatigue cracks can be predicted at the areas where peak stresses occur. For example, finite element

(FE) analysis based upon S-N curves has been utilized to study the fatigue properties of hybrid reconstruction plates used for treatment of mandible segmental defects [370]. In another study, Antoniac et al. [384] developed the FE model to quantify the maximum principal stress in the fixation plate, thereby predicting the fatigue lifespan on the basis of the S-N curve obtained from the published literature. Using a similar numerical approach, Chen et al. [385] estimated the fatigue limit of a locking compression plate used for stabilizing a fractured femur, which exhibited reasonably good agreement with the experimental data.

Nevertheless, these conventional S-N based FE techniques cannot predict the fatigue crack patterns, nor reveal the relationship between crack growth process and loading cycles. To overcome this limitation, conventional FE models are adopted to enable simulation of crack initiation and propagation inside a structure as per fracture mechanics [386, 387]. One possible way is to re-mesh the crack tip by assigning the elemental boundary to be a crack front [388], which often necessitates a sufficiently dense mesh near the crack tip. This can be performed by using some commercial programs, such as FRANC3D, which allows for modelling cracking process. In this regard, Mangardich et al employed FRANC3D to mimic the fatigue crack propagation of a compressor blade in an aircraft engine [389]. Loureiro-Homs et al. predicted the crack growth behaviours under thermomechanical fatigue conditions using FRANC3D, which showed reasonably good agreement with the experimental data [390]. However, re-meshing can be computationally expensive in particular for 3D structures. Furthermore, the frequent change in mesh topology during the course of crack tip extension could affect the simulation accuracy [381, 388].

To overcome the complications associated with conventional FE-based approaches, the eXtended Finite Element Method (XFEM) can be implemented to more effectively model

crack propagation without constantly re-meshing, so that the crack location and geometry can be easily determined without altering the initial mesh. XFEM also enables to eliminate the need for placing singular or Barsoum elements for capturing the singularity at crack tip as required in conventional FEM [101, 381]. Attributable to these advantages, the XFEM has been extensively used to simulate crack propagation for a wide range of materials and structures in literature [86, 104, 106, 109].

More recently, a few studies have employed XFEM to model fatigue crack growth (FCG) in several engineering applications [381]. For example, Nikfam et al. [388] evaluated high cycle fatigue crack growth in steel welded T-joints using XFEM. In another study, Dirik and Yalcinkaya [391] adopted XFEM to predict the fatigue life of 7075-T6 aluminium alloy specimens under mixed cyclic loading with variable amplitudes, which exhibited excellent correlation with the experimental results in terms of the cracking patterns and fatigue life (number of cycles to failure) [391]. Nonetheless, applications of XFEM for biomedical fatigue problems remain an open research question in literature to date.

This study aims to expand the XFEM modelling technique for biomedical applications by investigating fatigue characteristics of fixation systems used in orthopaedic surgery. The developed XFEM model is first validated through comparison with experimental data reported in literature. Then, two representative fixation plates that are used for stabilizing femur scaffolds and orofacial-maxillary reconstruction are explored, respectively. The present study demonstrates the effectiveness of XFEM for predicting the fatigue life and cracking process of such fixation plates commonly used in orthopaedics.

The remainder of the paper is organized as follows. Section 2 briefs the XFEM technique for fatigue crack propagation modelling. Section 3 is devoted to presenting three case studies

of fatigue characteristics, specifically a benchmark problem on fatigue failure of a compact tension specimen, a femoral osteofixation plate and a mandibular reconstruction plate. Section 4 offers discussion based upon the numerical results of these three case studies. Finally, section 5 draws some conclusions.

6.2 Materials and Methods

6.2.1 Fatigue modelling

The direct cyclic analysis module in Abaqus/Standard provides an effective modelling tool for generating stable responses of a structure subjected to cyclic loading. The cyclic loadings accumulate a stabilized response, called strain shakedown phenomena [136]. The conventional approach to generating this response is to apply cyclic loading repetitively to the model until a stabilized state is achieved, which can be however computationally expensive as it may require application of many loading cycles before a stabilized response is achieved. To avoid such high computational cost, the stabilized response is obtained by a modified Newton method in conjunction with a Fourier representation of the solution [139, 392], in which the truncated Fourier series of a displacement function $u(t)$ is expressed as [392],

$$u(t) = u_0 + \sum_{k=1}^n [u_k^s \sin(k\omega t) + u_k^c \cos(k\omega t)] \quad (6.1)$$

where n is the number of terms in the Fourier series and t is time. ω denotes the angular frequency. u_0 , u_k^s , and u_k^c are the unknown displacement coefficients associated with each degree of freedom.

At the end of each loading cycle, the corrections to the displacement Fourier coefficients, c_0 , c_k^s , and c_k^c , can be obtained; and the next displacement coefficients are updated as [392, 393],

$$u_0^{(i+1)} = u_0^{(i)} + c_0^{(i+1)} \quad (6.2)$$

$$u_k^{c(i+1)} = u_k^{c(i)} + c_k^{c(i+1)} \quad (6.3)$$

$$u_k^{s(i+1)} = u_k^{s(i)} + c_k^{s(i+1)} \quad (6.4)$$

Such updated displacement coefficients given in Eqs. (6.2)-(6.4) are used in the next iteration to obtain displacements at each instant of time.

Note that at a given point in the loading history, the stiffness at a material point remains unchanged when the stabilized solution is computed. Each of the solutions along the loading history represents a stabilized response of the structure, with a level of material damage at each point in the structure computed from the previous iteration. This process is repeated up to a time point in the loading history, at which a fatigue life can be assessed. In this way, the crack tip position and crack growth rate is updated continually throughout the iterative analysis.

In this study, damage initiation is estimated from the accumulated hysteresis energy per cycle, ΔW , in a stabilized state [139, 394]. The number of cycles to initiate a crack is thus given by [395, 396],

$$N_0 = A(\Delta W)^B \quad (6.5)$$

where A and B are the material constants, which can be determined via a fitting exercise by correlating with the corresponding experimental data [396, 397].

Once the crack has initiated, the maximum principal stress criterion is employed to determine the crack growth direction [392]. Crack growth is characterized by the stress intensity factor (SIF), K , at the crack tip in line with the Paris law [398, 399]. The range of SIF (ΔK) under cyclic loading with constant amplitude can be calculated as,

$$\Delta K = K_{max} - K_{min} \quad (6.6)$$

where K_{max} and K_{min} are the stress intensity factors corresponding to the maximum and minimum loads applied, respectively. The generalized Paris law can be expressed as [387, 400],

$$\frac{da}{dN} = C(\Delta K)^m \quad (6.7)$$

where a is the crack length and N the number of loading cycles. C and m are material dependent Paris' constant and Paris' exponent, respectively.

The Paris regime is bounded by the threshold SIF (K_{th}) and fatigue critical SIF (K_{fc}) values [387]. When ΔK is lower than K_{th} , the crack will not propagate; and once ΔK exceeds the K_{fc} value, the fatigue crack would grow at an accelerated rate, which could generally lead to an unstable crack. In the region with stable fatigue crack propagation, the crack growth rate (da/dN) is dependent upon the SIF range. At the time of failure, the number of cycles elapsed thus gives the fatigue life of the structure.

In addition, the SIF under sole failure modes is only capable of analyzing planar cracks under the uniaxial loading which is inapplicable of the case under mixed mode loadings. In order to evaluate non-planar crack propagation, mixed-mode fatigue crack growth was considered herein, which can be calculated based upon a user-specified criterion [398]. This study follows Nikfam et al. [388] in terms of an equivalent SIF range as,

$$\Delta K_{eq} = \sqrt{\Delta K_I^2 + \Delta K_{II}^2 + \Delta K_{III}^2 / (1 - \nu)} \quad (6.8)$$

where K_I , K_{II} , and K_{III} represent the SIFs in fracture modes I, II and III, respectively, ν is Poisson's ratio.

6.2.2 eXtended Finite Element Method (XFEM)

XFEM allows insertion of a crack by introducing additional degrees of freedom to the nodes belonging to the elements affected by the discontinuity. Depending on the discontinuation mode, two enrichment functions are commonly adopted, namely (1) a Heaviside discontinuous function, which models the jump of the displacement field along with the cracking faces in fully sectioned elements; and (2) crack tip function for modelling the near tip asymptotic field, which allows handling the stress singularity in the crack tip (or crack front region) [381].

The approach for enriching displacement field in XFEM can be briefly described as,

$$\mathbf{u} = \sum_{j=1}^n N_j(x) [\mathbf{u}_j + H(x)\mathbf{a}_j + \sum_{\alpha=1}^{ne(j)} F_{\alpha}(x)\mathbf{b}_j^{\alpha}] \quad (6.9)$$

where N_j represents the conventional shape functions associated with node j , $\mathbf{u}_j$ denotes the nodal displacement, $H(x)$ is the Heaviside function which is +1 on one side of the discontinuity and -1 on the other side of the discontinuity, $\mathbf{a}_j$ denotes the additional degree of freedom associated with the Heaviside function, $F_{\alpha}(x)$ is the crack tip function (see Eq. (6.10) below), $\mathbf{b}_j$ stands for the extra

degree of freedom associated with the crack tip function, and $ne(j)$ represents the number of $F_\alpha(x)$ for node j .

The crack tip function is obtained from the asymptotic displacement fields as,

$$F_\alpha(x) = \left[\sqrt{r} \sin\left(\frac{\theta}{2}\right), \sqrt{r} \cos\left(\frac{\theta}{2}\right), \sqrt{r} \sin\theta \sin\left(\frac{\theta}{2}\right), \sqrt{r} \sin\theta \cos\left(\frac{\theta}{2}\right) \right] \quad (6.10)$$

where r and θ are the polar coordinates in the local crack tip coordinate system.

As for the XFEM module in Abaqus, the crack tip function is used for modeling a stationary crack. Therefore, for modeling crack propagation, the near-tip asymptotic singularity given by Eq. (6.10) is not considered.

6.2.3 Level set representation of crack surface

The Level Set Method (LSM) is employed here to track the cracking path in 3D space. Two quasi-orthogonal functions, namely $\phi(\mathbf{x}, \tau)$ and $\psi(\mathbf{x}, \tau)$, are utilized to express the geometry of the cracking surfaces. The first function, $\phi(\mathbf{x}, \tau)$, defines the crack surface, where $\mathbf{x}$ and τ denote the point in space and time domain, respectively. The second function, $\psi(\mathbf{x}, \tau)$, is used to construct an orthogonal surface, so that the intersection of these two surfaces gives the crack front.

Abaqus XFEM module allows to store the results relating to both the functions with full details of element types and location of the nodes. Such information can be used to extract the progression of the crack surface throughout the analysis using custom-developed code to implement the following procedures:

1. All the elements associated with the crack are identified by noting where the elemental output STATUSXFEM is non-zero.
2. Level set PHILSM quantities are extracted at each node of the previously identified elements.
3. The level set $\phi(\mathbf{x}, \tau)$ results are interpolated across the domain of the elements using the shape function applicable to that element.
4. Zero crossings are located on the edges of the elements; the crack surface within one element spans these zero crossings.

5. The total area of cracked surfaces is determined as the aggregate of all the elemental crack surfaces.

The above procedures are performed for each step of the XFEM fatigue analysis, which allows the evolution details of the crack to be studied as the simulation progresses.

6.3 Demonstrative examples

In this section, one engineering and two biomedical examples are presented for fatigue analyses. The first deals with a benchmark engineering problem involving a modified compact tension specimen, which is used to validate the XFEM analysis of fatigue crack growth (FCG) and fatigue life. The second example studies the fatigue failure of a femoral osteofixation plate; and the third example investigates the fatigue behaviour of a fixation plate used for mandibular reconstruction.

6.3.1 ASTM modified compact tension specimen

In this example, the experimental study reported by Lu et al. [401] on the ASTM modified compact tension specimen is used for validation of XFEM fatigue analysis. The geometry and dimensions of the modified compact tension specimen with an initial crack length of $a_0 = 10.5$ mm is illustrated in **Figure 6.1**. The structure was modelled as a plane stress problem with a plate thickness of 5 mm. In this 2D FE model, a mesh size of 0.4 mm was used after a convergence study, where the total number of quadrilateral linear elements is 17,317, with 35,438 degrees of freedom. The plate was made of Al 7075-T6, whose material properties are summarized in **Table 6.1**.

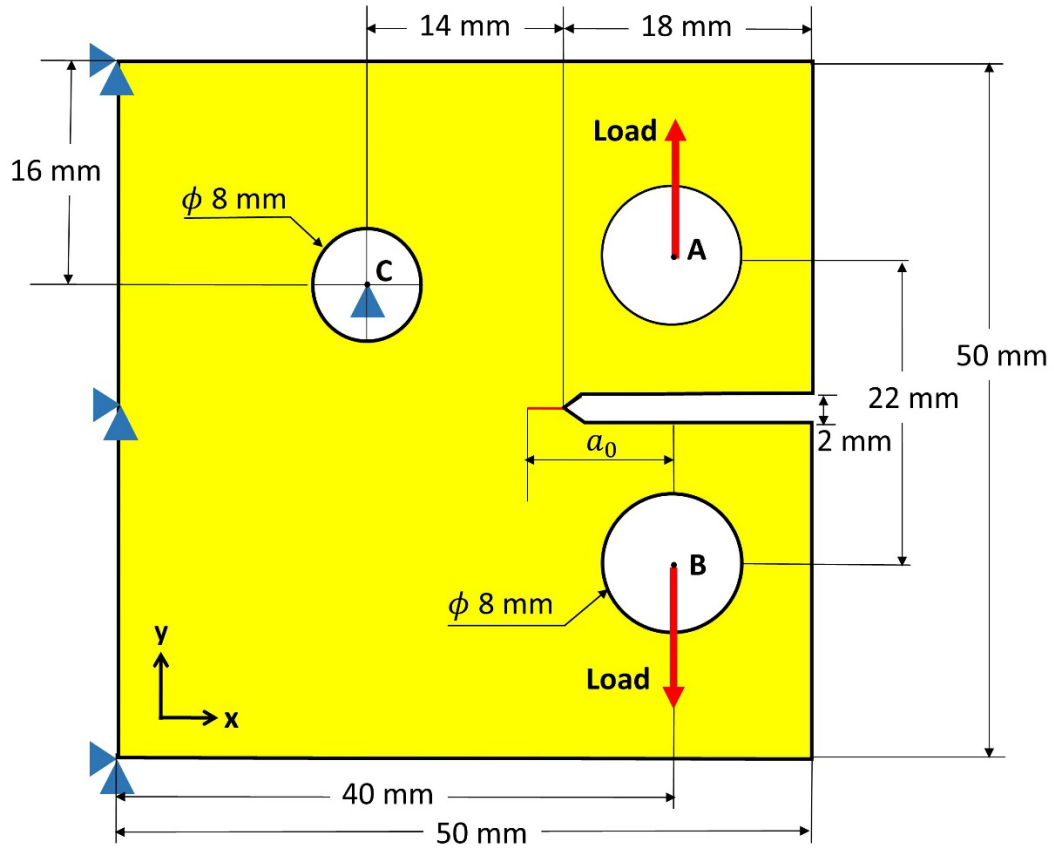


Figure 6.1: Schematic of the ASTM modified compact tension structure illustrating the loading and boundary conditions as reported by Lu et al. [401].

Table 6.1: Material properties for the ASTM specimen reported by Lu et al. [401].

Young's Modulus E (MPa)	Poisson's ratio ν	Yield stress σ_Y (MPa)	Fracture toughness K_{Ic} (MPa $\sqrt{mm}$)	C (mm/(cycle * MPa $\sqrt{mm}$))	m
71.7×10^3	0.33	516	730	1.2×10^{-9}	3.0

Concerning the loading and boundary conditions, a constant cyclic load, with a lower bound of 200 N and an upper bound of 2,000 N, was adopted herein [391]. The loads were applied oppositely on the centres of hole A and B (**Figure 6.1**); and the centre points were

connected to the region about the holes by means of a coupling connection. The left edge of the specimen was fully constrained (shown as the blue triangles in **Figure 6.1**) in all the translational directions, while the specimen was constrained in the y direction at the center of hole C.

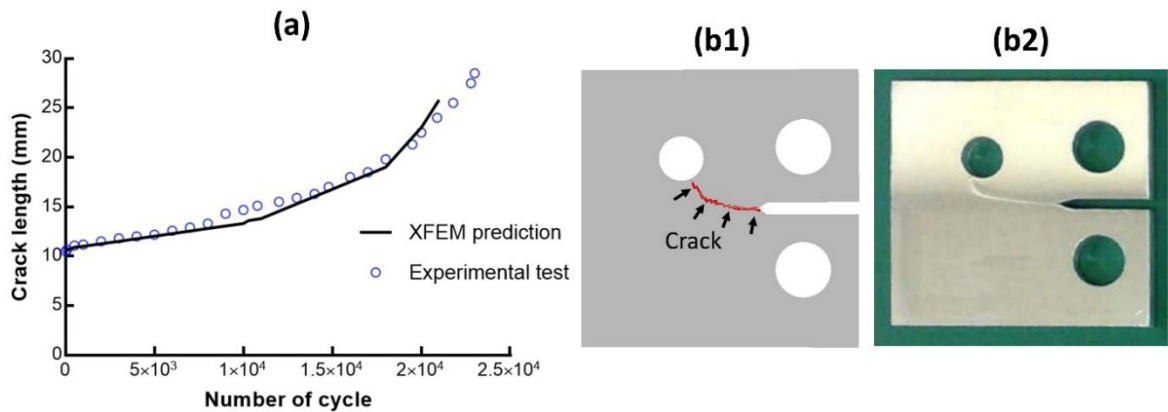


Figure 6.2: (a) The correlation between simulated and experimental fatigue life of the modified compact tension specimen [401]; (b1) the predicted cracking path and final rupture pattern; (b2) experimentally observed crack path for the compact tension structure under the constant cyclic loading [401].

The fatigue cracking length versus the number of loading cycles obtained from the simulated and experimental results are compared in **Figure 6.2(a)**. Despite some minor discrepancies between the predicated and the experimental results (possibly due to the material assumptions and test conditions), fairly reasonable agreement between them can be observed, as shown in **Figure 6.2(a)** [401]. According to the simulated cracking path shown in **Figure 6.2(b1)**, hole C affected the crack propagation and has clearly drawn the crack towards it, which is consistent with the experimental observations shown in **Figure 6.2(b2)**, while there is marginal deviation between the simulated and experimental cracking paths in

the end towards C. Therefore, the effectiveness of XFEM for simulating the FCG life and cracking path is well demonstrated through this benchmarking example.

6.3.2 Femoral osteofixation plate

The second example investigated the fatigue fracture behaviour of a typical femoral osteofixation plate. Specifically, a surgical blade plate (10 hole condylar plate, DePuy Synthes, UK) and Synthes Deputy VET 4.5 mm self-tapping cortical screws (VS402.036) were utilized to stabilize bone defects/fracture created in a composite femur model (4th generation composite, Sawbones, USA) [253].

In the numerical simulations, three different case scenarios were considered here: (1) a transversely fractured femur, namely Model-A, (**Figure 6.3(a)**); (2) a segmental defect in the femur treated by a tissue scaffold, namely Model-B, (**Figure 6.3(b)**); and (3) a segmental defect in the femur treated by a tissue scaffold which was filled with newly regenerated bone, namely Model-C, (**Figure 6.3(c)**). In the first case scenario (as depicted in **Figure 6.3(a)**), a transverse bone fracture was modelled, where a thin layer of soft matter was placed in the fracture gap to simulate the hematoma tissue [385]. The tissue scaffold used in the second case scenario involved a 3D orthogonal structure (as shown in **Figure 6.3(d)**), which was designed in SolidWorks and further 3D printed (Objet Eden260VS, Stratasys, USA)) in a commercial photopolymer VeroWhitePlus (RGD 835) for experimental testing [253].

To create the 3D numerical models, the CAD model of the composite femur bone was obtained from the Pacific Research Labs (part number 3908, Sawbone, USA). According to the manufacturer (Sawbone, USA), an optical white light scanner (3D3 Solutions HDI Advance R3, GOMEASURE3D, Amherst, VA, USA) was used to digitize the surface of the

cortex and core of the femur separately (FlexScan3D, LMI Technologies (USA) Inc., U.S.A.), followed by surfacing them using Rapidform XOR3. Then, the core and cortex were assembled into the final solid model of femur in SolidWorks. The CAD models of the surgical plate and screws were created based upon measurements of the actual devices used in the experiments.

The assembled models were then imported into Abaqus (ABAQUS, Inc, Providence, RI). A frictional contact with a frictional coefficient of 0.4 was assigned for the interfaces between the screws and the plate [385]. The contact between the screws and bone was considered to be tied. The interface between femur and supporting resin die was also assumed as fully bonded, where relative slip between each component was prevented. The constant cyclic load, with lower bound of 0 N and upper bound of 950 N was applied to the femoral head along the stance direction (i.e. 7° from the anatomical femur axis), as shown in **Figure 6.3(e)**, which represented the physiological standing posture [402-404]. To control the computational cost, the cracking region was only applied to the plate in XFEM. A mesh convergence study was performed to balance the simulation accuracy and efficiency, in which the total number of linear tetrahedron elements was 361,697 with 1,085,091 degrees of freedom.

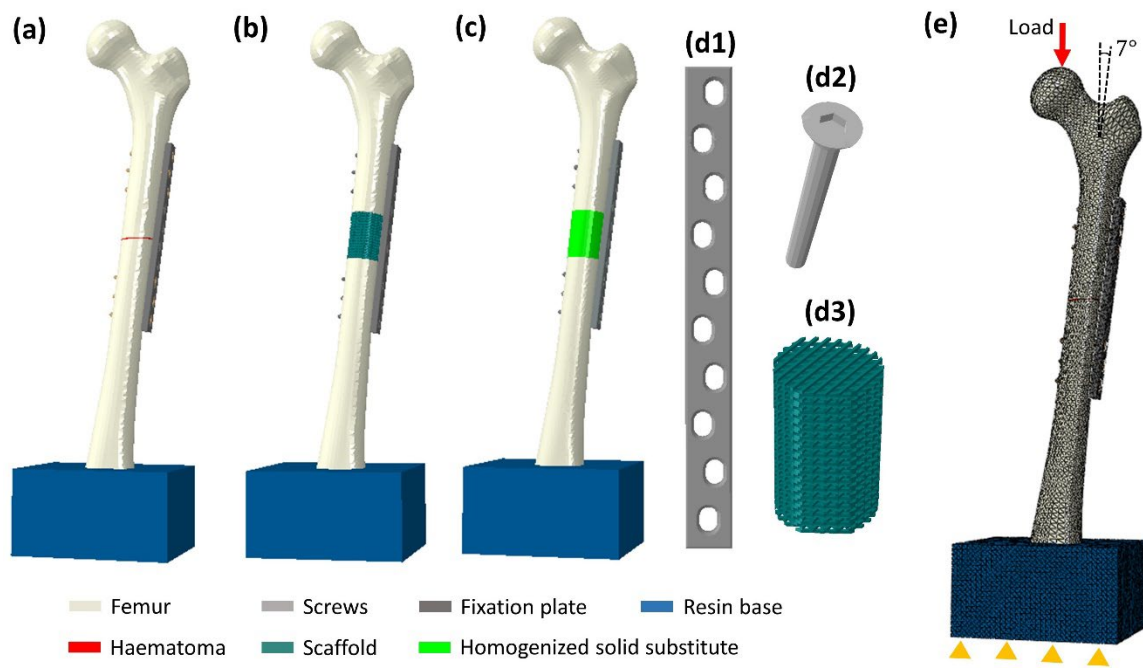


Figure 6.3: The numerical models related to three different treatment scenarios of femoral fracture/defects with the same osteofixation plating system. (a) Model-A: a transversely-fractured femur in which a thin layer of soft connective tissue (hematoma) was modelled in the cracking gap; (b) Model-B: a femur with a segmental bone defect implanted using a tissue scaffold; (c) Model-C: a femur with a segmental bone defect filled with a homogenized composite substitute which presented both the scaffold and the newly formed bone inside scaffold; (d1) fixation plate; (d2) simplified screw models; (d3) tissue scaffold; (e) loading and boundary conditions. The red arrow shows the force applied on the femur head and the yellow triangles represent the kinematic boundary condition on the distal end of the femur model.

In this study, the osteofixation plate and the screws were made of 316LR stainless steel. Each component of the numerical models was assumed to be homogenous and isotropic with

the material properties summarized in **Table 6.2**. Regarding the hysteresis energy criterion, material constants A and B can be obtained under continuous strain-controlled push-pull tests; and a value of $6.42 \times 10^6 \text{ MPa}^{-B}$ for parameter A and a value of -6.52 for parameter B were used in this study [395]. The Paris' constants C and exponent m were determined by mode I fatigue crack growth (FCG) experiments, which were given to be 4.051×10^{-8} and 2.348, respectively, and the threshold stress intensity factor K_{th} was determined as $6.7 \text{ MPa}\sqrt{m}$ [398, 405].

Table 6.2: Material properties of each component used in the numerical simulations related to the femur treatment models with the osteofixation plate system [253, 385].

Materials	Young's Modulus E (MPa)	Poisson's Ratio ν	Yield Strength σ_Y (MPa)	Ultimate Tensile Strength σ_{TS} (MPa)	Fracture Toughness K_{IC} (MPa $\sqrt{m}$)
Plate	200×10^3	0.3	295	582	71.26
Screw	200×10^3	0.3	295	582	71.26
Cortical	16.7×10^3	0.26	-	-	-
Cancellous	155	0.26	-	-	-
Hematoma	5	0.49	-	-	-
Scaffold	1.5×10^3	0.3	-	-	-
Resin	3×10^3	0.3	-	-	-

To simulate bone ingrowth into the scaffold in Model-B, the entire defect was assumed to be filled with a homogenized substitute medium which represented both the polymeric scaffold (VeroWhitePlus (RGD 835)) and the newly formed bony tissues within the scaffold. The effective Young's modulus of the homogenized substitute was obtained as,

$$E_{effective} = E_{polymer}V_{polymer} + E_{bone}V_{bone} \quad (6.11)$$

where $E_{polymer}$ and E_{bone} were Young's moduli of the polymeric material of scaffold (VeroWhitePlus (RGD 835)) and the new bony tissue, respectively. $V_{polymer}$ was the volume fraction of the polymeric material (i.e. the scaffold), which was 0.3 for the given scaffold (i.e. porosity of 70%). In this study, the newly formed bony tissue was assumed to fill only half of the void volume within the scaffold [406], therefore, the volume fraction of newly formed bone tissue, V_{bone} , was taken as 0.35.

To validate the scaffold-femur model, an *in-vitro* mechanical tests were first performed, in which a 3D digital image correlation (DIC) system was employed for measuring the full-field surface displacements and strains in the fixation plate concerned. **Figure 6.4(a1)** illustrates the experimental set-up for the DIC system. Similarly to our previous study [253], speckle patterns were randomly sprayed on the surface of the specimens, and a high-speed camera (50 mm lenses with 20 mm distance rings, GOM GmbH, Germany) was used to capture consecutive images during the test. The surface displacements and strains can be calculated by correlating the deformed images taken by the camera during the loading process with respect to the reference image. For the plate used in the nominated model (Model-B), **Figure 6.4(a)** compares the y-directional displacement and strain results obtained from the numerical simulations and the experimental DIC test. In spite of some discrepancies between the *in-vitro* and *in-silico* strain contours, the majority of them exhibited fairly good agreement, thereby demonstrating the FE modelling accuracy of scaffold-treated femur reconstruction system for the fatigue analysis.

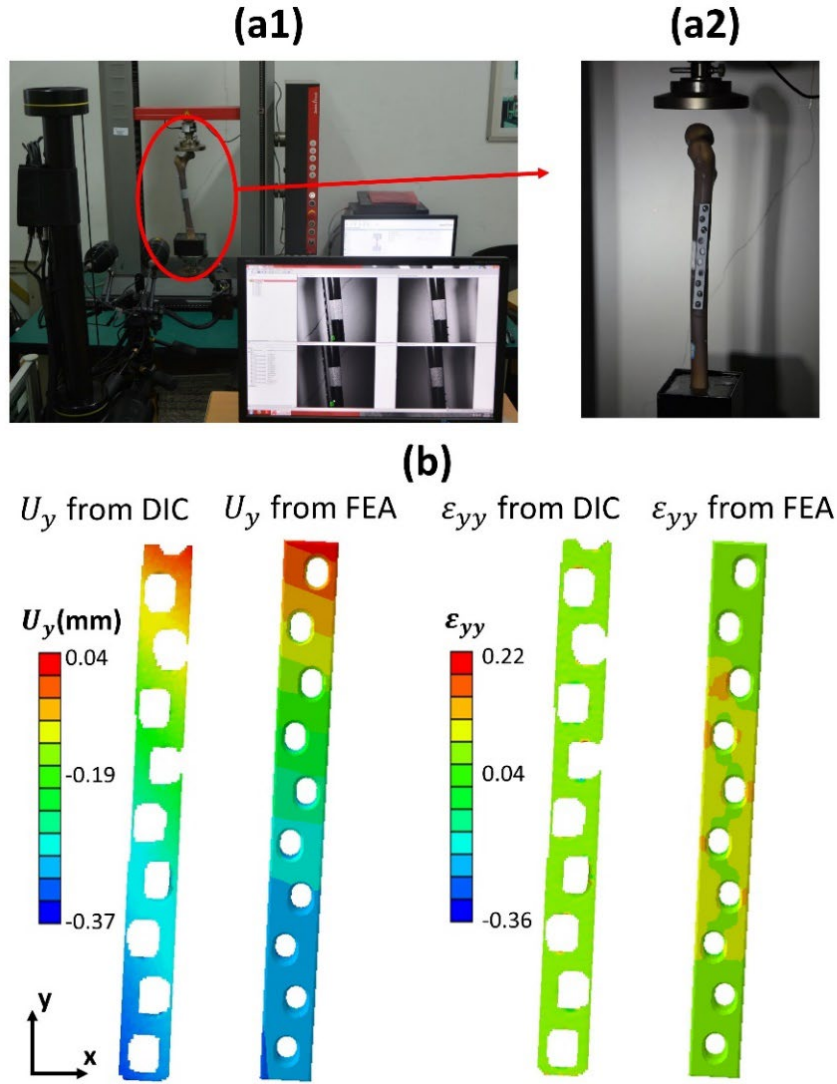


Figure 6.4: (a1) The digital image correlation (DIC) system set-up for measuring surface displacement and strain developed in the fixation plate; (a2) The close view of the assembly of Sawbone femur, scaffold and plating system for the experimental testing; (b) The contours of y-directional displacement and strain in the fixation plate in Model-B, obtained from the 3D DIC technique and XFEM, respectively.

Figure 6.5 compares the maximum principal stress (MPS) contours in the osteofixation plate system used in each case in this example. It can be observed that, in all the models, the majority of the regions in the femur experienced compressive MPS except for the femur neck. On the other hand, the maximum tensile MPS magnitudes are largely concentrated in the plate and the screws. The region with the highest tensile MPS was identified in the plates, which occurred in the margin of screw holes as indicated by the arrows in **Figure 6.5**. The comparison between these three different scenarios indicated that the plates used in Model-A and Model-B experienced the lowest and the highest peak MPS, respectively (i.e. 262.23 MPa in Model-A vs 483.69 MPa in Model-B). Moreover, the peak MPS experienced by the plate used in Model-C was 348.27MPa, which was substantially lower than that of Model-B, indicating the significant effect of new bone formation within the scaffold. The results also show that while the magnitude of MPS in the plates was strongly affected by the presence of the segmental bone defect and the newly formed bone, these three numerical models exhibit similar stress distribution patterns.

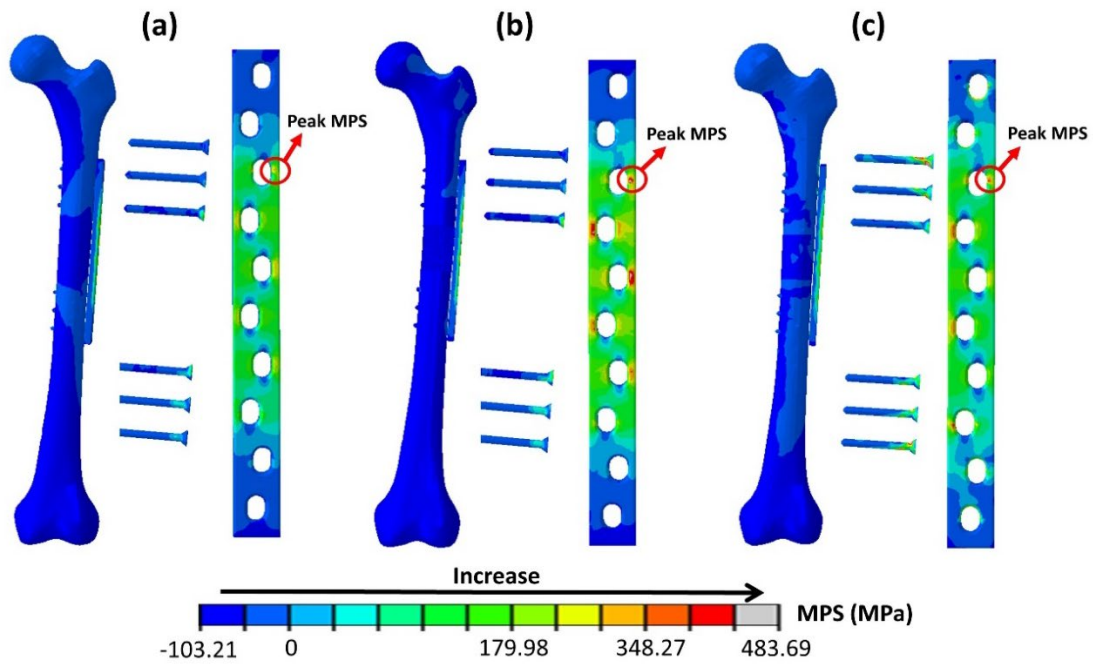


Figure 6.5: Maximum principal stress (MPS) in the femoral osteofixation plate system used for: (a) the transversely-fractured femur; (b) the femur with a segmental bone defect treated by a tissue scaffold; (c) the femur with a segmental bone defect filled with a homogenized substitute construct representing both the scaffold and the newly formed bone inside the scaffold.

Based upon the XFEM fatigue analysis, **Figure 6.6(a)** compares these three plates used for treating the transverse fracture and segmental defect in terms of evolution of cracking surface area with respect to loading cycles. It can be observed that Model-A exhibited the longest fatigue life (14,017,301 cycles), followed by Model-C (388,735 cycles) and Model-B (192,559 cycles). Interestingly, the cracking surface area in Model-B was radically elevated when the cyclic loading reached 25,107 cycles, followed by a plateau in the cracking area regardless of increase in loading cycles. Following the plateau, there was a significant increase in the cracking area when the number of loading cycles exceeded 109,287. At this stage, the final fracture could be seen in the plates (as depicted in **Figure 6.6(c)**). It can be

seen that Model-C exhibited a longer lifespan prior to crack initiation within the plate (61,051 cycles). By comparing the number of loading cycles up to the final failure, the plate in Model-B exhibited relatively lower fatigue life, reported as 192,559 cycles, in comparison with Model-C (388,735 cycles).

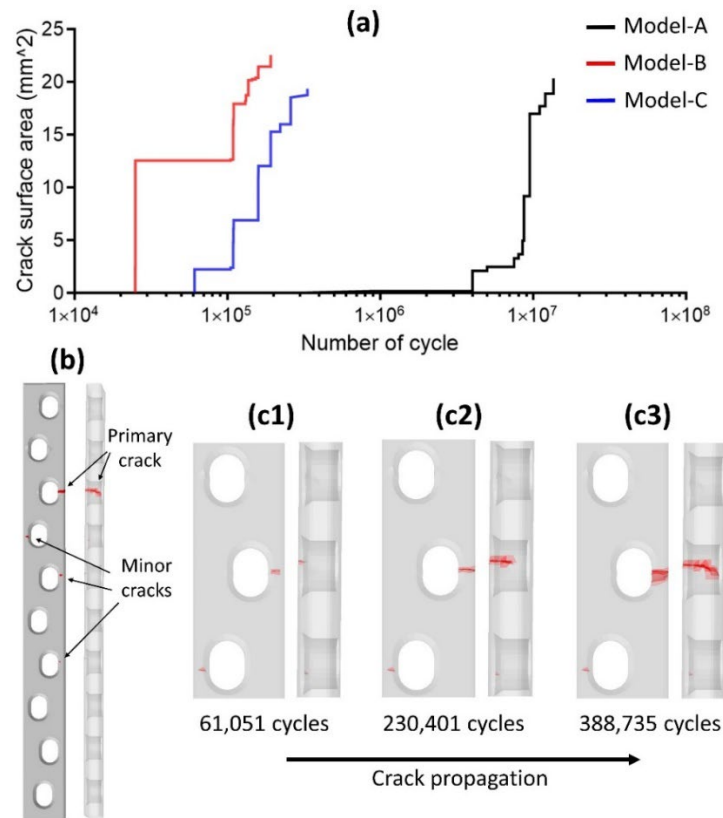


Figure 6.6: (a) Plots of simulated cracking surface areas versus number of loading cycles; (b) Typical fracture pattern in the femoral osteofixation plate (Model-B); and (c) Simulated crack propagation path (Model-B): c1) at 61,051 cycles, (c2) at 230,401 cycles, (3) at 388,735 cycles.

In a physiologically normal adult, the lower limb can be loaded up to 5,000-7,000 times per day [372, 407]. In this example, if 5,000 cycles per day was assumed for the patient; the

fatigue life of the plates used in Model-B and Model-C could be pronounced as 39 and 78 days, respectively. The results indicated that subsequent bone healing and tissue ingrowth (i.e. 50% new bone formed inside the scaffold) could considerably increase the longevity and fatigue life of the plating system.

From **Figure 6.6**, it can be seen that Model-A (i.e. the transversely-fractured femur) exhibited significantly longer fatigue lifespan than the other two major defect models. For the plate used in Model-A, the crack was initiated at 894,501 cycles and a complete fracture may not be observed until 1.4×10^7 cycles, which corresponded to 2,800 days of fatigue life. Relatively similar fatigue life (more than 2,000 days) was reported in [385], which investigated the fatigue life of a femur fixation plate through the S-N curve method.

The crack growth in all these investigated femoral osteofixation plates were found to be similar and stable, and the representative crack patterns (as exemplified from Model-B) are depicted in **Figure 6.6**, where the simulated crack propagation path in the plate is shown in **Figure 6.6(c)**. Generally speaking, the crack was initiated after a limited number of loading cycles and progressively extended with increased loading cycles until final fracture of the plate. It can be seen that multiple cracks could initiate from the thinner regions around the plate holes (**Figure 6.6(c1)**). Although multiple cracks initiated almost at the same time, only one crack propagated extensively as the load cycles increased, namely a primary crack; and ultimately, the primary crack propagated through the entire thickness of the plate and caused the plate to fracture. Nevertheless, the other cracks, namely minor cracks, were fairly stable and did not appear to grow much with the increase in loading cycles in this example.

6.3.3 Mandibular reconstruction plate

The third example investigated the fatigue behaviour of a fixation plate used for mandibular reconstruction. To establish the numerical model, the 3D mandible model was created based upon the computed tomography (CT) images of a 66-year-old male patient by using commercial software ScanIP (Simpleware Exeter, UK). After segmentation, surface smoothing and refinement, the 3D solid model was imported to Abaqus. This example considered three different case scenarios for the mandible: (1) a mandible model with a major segmental bone defect on the right side, namely Model-1 (**Figure 6.7(a)**), (2) the reconstructed mandible with fibula free flap (FFF) at the initial stage [408], namely Model-2 (**Figure 6.7(b)**), and the fully healed reconstructed mandible for a comparison purpose, namely Model-3 (**Figure 6.7(c)**). The titanium mandibular reconstruction plate and screws were modelled in SolidWorks based upon the standard design from a commercial system (Synthes, Solothurn, Switzerland) [408]. The models were imported in Abaqus for assembling the complete FE models. Finally, the FE models were meshed by linear tetrahedron elements after a convergence test similarly to our previous studies [408-410].

The increase in biting force magnitude may occur when the biting location moves from the anterior to posterior teeth, and the molar tooth may be able to carry the maximum biting force, which is typically around 125N for the patients with mandible resection [370, 375]. In the case of a fatigue failure scenario, however, the cyclic loading magnitude may not necessarily reach the maximum 125 N force. In line with the literature [370, 374], the cyclic load was assumed to have a lower limit of 0 N and upper limit of 80% of the maximum occlusal loading, which is 100 N. Our recent clinical study on the muscular force measurement confirmed such a loading level in this specific patient [410]. Thus, as shown in

Figure 6.7(d), an oblique load of 100N is applied on the left second molar (30° in the buccolingual direction, inclination to the normal axis of the occlusal surface in the second molar) [411]. The temporomandibular joint was fully constrained [370, 411]; and the interfaces between the plate and screws, as well as the interface between the screws and the mandible bone were considered to be fully bonded after a certain period of osseointegration [370, 375].

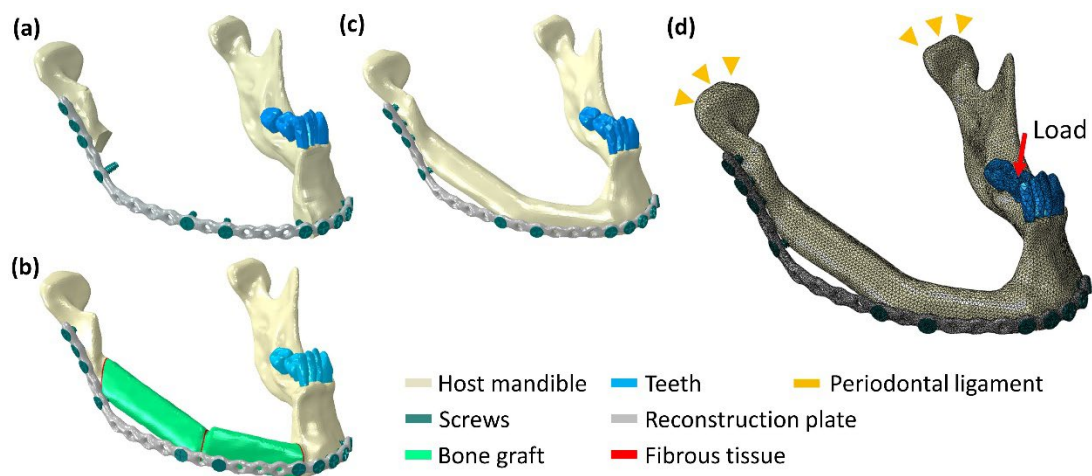


Figure 6.7: 3D FE mandible models with a reconstruction fixation system. (a) The mandible model with segmental defect and bridged by a fixation plate (Model-1); (b) the reconstructed mandible with fibula free flap (FFF) at the initial stage (Model-2); (c) the fully healed reconstructed mandible with fixation plate system (Model-3); (d) loading and boundary conditions. The red arrow shows the applied occlusal force on the left second molar, and the yellow triangles represent the constraints around the temporomandibular joints.

Since this example focuses on the fatigue fracture in the reconstruction plate, the mandibular bone was approximated to be a homogeneous, isotropic and linear elastic material

[86, 104, 412]. The surgical reconstruction plates and screws were made of titanium ASTN F67/2 (Ti grade 2), which was also considered to be isotropic and linear elastic in the fatigue analysis [375]. The mechanical properties of all the materials involved in the numerical simulations are summarized in **Table 6.3**. The material constants A and B , which are used in the hysteresis energy criterion, can be obtained from standard material testing, and a value of $5.17 \times 10^5 \text{ MPa}^{-B}$ for parameter A and a value of -2.37 for parameter B were used in this study [395]. According to Kumar et al. [413], the Paris' constant C and exponent m were taken as 5.88×10^{-8} and 3.17 for the titanium alloy, respectively; and the threshold stress intensity factor K_{th} was determined as $8.3 \text{ MPa}\sqrt{m}$.

Table 6.3: Material properties of the simulated mandible and reconstruction plate system [36, 37].

Materials	Young's Modulus E (MPa)	Poisson's Ratio ν	Yield Strength σ_Y (MPa)	Ultimate Tensile Stress σ_{TS} (MPa)	Fracture Toughness K_{IC} (MPa·m ^{1/2})
Plate	105×10^3	0.3	276	445	29
Screw	105×10^3	0.3	276	445	29
Mandible	12.2×10^3	0.3	-	-	-
Bone Graft	1,650	0.3	-	-	-
Fibrous tissue	200	0.4	-	-	-
Tooth	80×10^3	0.28	-	-	-
PDL	70	0.45	-	-	-

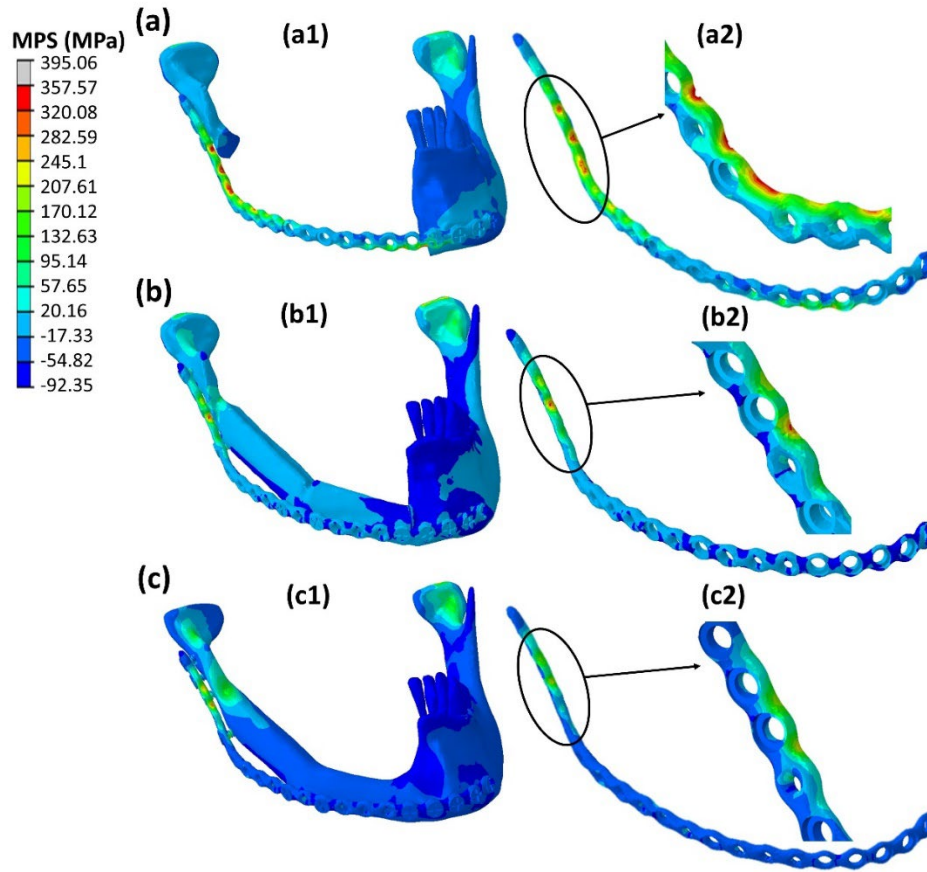


Figure 6.8: Maximum principal stress (MPS) contour of mandibular reconstruction system with the fixation plate. (a) The mandible with a segmental defect (Model-1); (b) the reconstructed mandible with FFF at the initial stage (Model-2); (c) fully healed reconstructed mandible model (Model-3). (a1), (b1) and (c1) show the overall stress distribution; (a2), (b2) and (c2) present the stress contour in the plate.

Figure 6.8 compares the MPS distributions in these three mandibular reconstruction cases (namely Model-1, Model-2 and Model-3). In general, it can be seen that the stress magnitude in the mandible was relatively lower (as displayed in **Figure 6.8(a1)** (b1) and (c1)) than those in the screws and plate; and the region with the highest MPS values can be found

in the reconstruction plate. Under the same occlusal loading condition, Model-1 exhibited the highest peak MPS (395.06MPa) in the plate, followed by the reconstructed mandible with FFF at the initial stage (335.44MPa), and the fully reconstructed mandible (Model-3) (248.71 MPa). Not only did the bone defect influence the magnitude of MPS, but it also altered the stress distribution in the reconstruction plates, as illustrated in **Figure 6.8(a2)** (b2) and (c2). Such a bone defect caused the stress to be concentrated on the edge of the holes near the bone defect margins (the top surface on the distal side and bottom surface on the proximal side) in the reconstruction plate. According to **Figure 6.8(b2)**, however, the area with an intensified stress was found to be slightly migrated towards the distal side. In addition, the plate on the fully reconstructed mandible (Model-3) was seen to have a more evenly distributed stress pattern, which almost eliminated the stress concentration from the edge of the holes as shown in **Figure 6.8(c2)**.

Figure 6.9(a) describes the relationship between cracking surface area and the number of loading cycles in these three models. The fully reconstructed mandible group displayed a more gradual tendency of crack propagation with respect to increase in loading cycles, in comparison with the other two models. The simulated crack in the fully reconstructed mandible initiated at 15,010 cycles; and after a few abrupt jumps of the cracking surface area, the reconstruction plate finally fractured after 338,833 cycles. On the contrary, the plate in Model-1 experienced an initial crack as early as 5,001 cycles, and then exhibited a dramatic rise in the cracking area at 15,717 cycles, followed by the final fracture after 26,788 loading cycles. Although the plate in Model-2 had a similar lifespan in crack initiation (at 7,301 cycles), it had a much longer fatigue life (78,598 cycles) to final fracture than Model-1,

In the literature, it was reported that an individual exhibits chewing and swallowing equivalent to three pieces of gum per day, with summation of swallowing time of around 10-min duration, at a chewing rate of about 60 cycles per minute [370]. This is equivalent to 600 cycles per day and approximately 2×10^5 cycles per year. In line with this estimation, the fatigue life of the fixation plate was only 1.6 months (around 48 days) in Model-1 and 4.3 months in Model-2. In contrast, the plate for fully reconstructed mandible (Model-3) could increase the fatigue lifespan up to 20.4 months.

Figure 6.9(b) compares the crack location and path of these three different models. For model-1, the crack originated near the distal side of the segmental defect margin, from the top surface of the plate; and then propagated downwards until it passed through the plate thickness. As for Model-2 and Model-3, the crack also initiated from the distal side of the plate, but the adjacent hole in the plate considerably affected the cracking path and led it to extend towards the hole. By comparing the cracking paths in Model-2 and Model-3, it is found that although the crack path was affected by the adjacent hole, it still propagated across the entire thickness of the plates in Model-2. In Model-3, the crack started from the top surface of the plate in the fully reconstructed mandible model, but passed through half the plate thickness and finally reached to the inner surface of the adjacent hole.

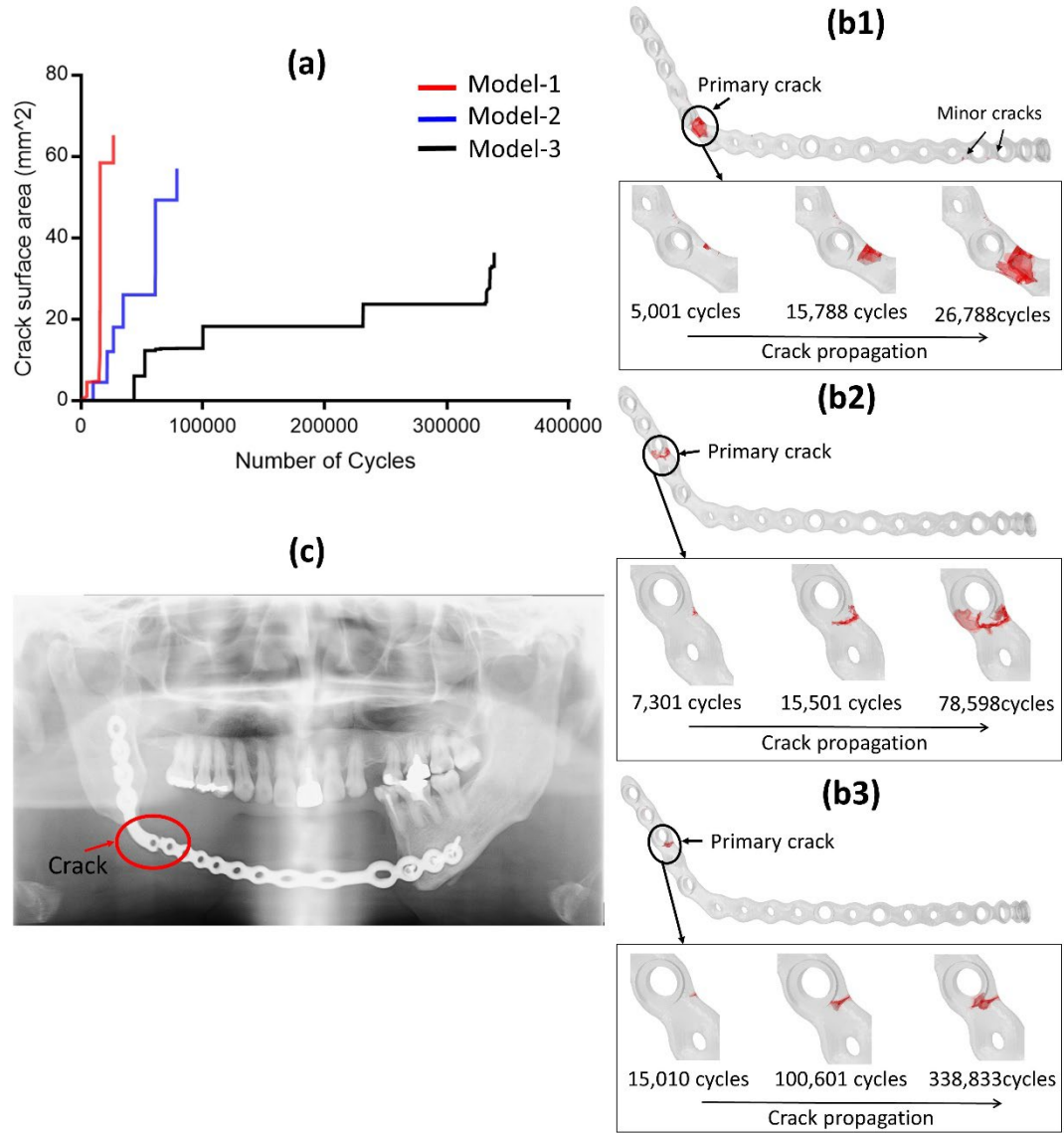


Figure 6.9: (a) The growth of crack surface area versus number of cycles obtained from the XFEM fatigue analyses for the three models considered; (b) simulated crack patterns and corresponding propagation path in the mandibular plates with different mandibular reconstruction conditions. (b1) Model-1; (b2) Model-2; (b3) Model-3. (c) the clinical case of fracture in titanium reconstruction plate.

Figure 6.9(c) shows a radiograph image of a clinical case where a titanium reconstruction plate fractured in some stage of the treatment. It can be seen that while there is

some discrepancy due to the bone defect and surgical strategy, the simulated rupture pattern and location (**Figure 6.9(b1)**) exhibited reasonable correlation with the clinical X-Ray diagnosis, which is near the distal side of segmental defect margin.

6.4 Discussion

A fixation system can play a key role in postoperative stabilization of fracture/defect sites for treating injured or diseased bones, directly contributing on long term clinical success [370, 377]. Not only does the fixation system support the system stability, but it is also involved in the subsequent healing and bone remodelling over time, meaning that longevity of a fixation system can be decisive in such surgical procedures [373, 414]. This study investigated the underlying biomechanical causes of fatigue failure in fixation plates through multiple case studies, in which the cracking paths and fatigue life of the fixation plates were evaluated for the first time through the novel XFEM-based approach presented.

To validate the XFEM-based approach, an engineering benchmark problem of an ASTM modified compact tension structure was analyzed first, which demonstrated excellent correlation between the XFEM-based simulation results and experimental data reported in [401], as shown in **Figure 6.2**. The ASTM compact tension specimens have been extensively used in the fracture and fatigue analyses in literature, owing to its capability in determining the stress intensity factor (SIF), K , which plays an important role in determining fatigue crack growth rate [391, 415, 416]. For example, Bergara et al. [387] employed the compact tension models to investigate the SIFs along the crack front under a mixed mode of cyclic loadings, and their simulation results exhibited good agreement with the analytical solutions provided by ASTM. Nevertheless, one limitation of the presented benchmark problem is that the

compact tension model has not specifically considered the effect of short crack size. Some literature studies indicate that the behaviour of short crack growth can be rather complex, in which wide-ranging factors, such as materials microstructure, dislocation plasticity, and crack size dependent short crack threshold, would have a strong influence on the short fatigue crack propagation [417, 418]. Therefore, the short cracks normally exhibited a higher crack growth rate compared to long cracks with the same range of stress intensity applied [418]. Further studies might be required to improve the proposed numerical framework by including the crack size effect.

Furthermore, the effectiveness of the presented XFEM-based approach for fatigue analyses was demonstrated by considering two widely used orthopaedic fixation plates. As shown in **Figure 6.5** and **Figure 6.8**, the location of maximum principal stress (MPS) concentration identified by the XFEM correlated well with the origin sites of the cracks (**Figure 6.6** and **Figure 6.9**), implying that the stress concentration-led crack initiation was driven by tensile rather than compressive stress. In both these two representative clinical examples presented for the femoral osteofixation and the mandibular reconstruction plates, the tensile stresses in the fixation plates were found to be generated from flexure of the fixation plates under the physiological loadings. For example, in the femoral osteofixation plate, the cracking sites were observed near the screw holes on the plates. This is due to the fact that the plate experienced substantial bending stress induced by the physiological loading whereas the screw holes presented a thinner plate margin near the holes with much less material to bear such complex loading, thereby leading to significant stress concentration near the holes [374]. Furthermore, the presence of holes led to local stress concentration due to a thinner margin in the plate, influencing the cracking path [419]. In the course of the

fatigue crack propagation, a higher stress concentration could vary and grow the crack path towards the adjacent hole.

Figure 6.6(a) and **Figure 6.9(a)** demonstrated the evolution of the cracking surface area with respect to increase in loading cycles. It can be seen that the crack growth curves included vertical and horizontal segments. This is due to the fact that the crack length was quantified to be crossing the full element mesh in XFEM. The combination of a finite crack advance with increase in loading cycles gives rise to the near-vertical graph segments, while the horizontal sections refer to that increase in loading cycles does not clearly propagate crack in this stage. By comparing the fatigue life for the different femoral fixation plates at several time points during healing, e.g. Model-B and Model-C, the XFEM results suggested that an appropriate healing and remodelling condition could significantly extend the fatigue life of the plates. This is due to the fact that bone ingrowth in the scaffold can considerably increase the stiffness and strength of the overall tissue construct in the course of the healing and regenerative process, which enables it to gradually take a certain percentage of total loading [420]. As a result, this enables to decrease the stress level in the fixation plate and thereby to increase its fatigue life.

Nevertheless, one limitation of the present femoral study is that only few representative time points were considered. The time-dependent tissue ingrowth during healing/remodelling process, e.g. the hematoma (soft connective tissue) transforming to soft callus (fibrocartilage) and hard callus (woven bone) in Model A, was not considered in detail [374]. However, the moduli of such soft tissues are generally much lower than those of the surround host bone, and the soft tissue layer is relatively thin, therefore, the effects of such soft tissues may not be significant [385].

Similar results can be found in the mandibular reconstruction case scenarios, in which the fixation plate in the fully healed FFF mandible exhibited a substantially longer fatigue life than the other two cases, indicating an increasing role in load-bearing capability played by the healed grafted bone. Concerning the effects of bone graft, the simulation results confirmed that the presence of grafted FFF bone could considerably alleviate the stress on the plate, thereby increasing its fatigue life from 1.6 months to 4.3 months. It could be explained by the bone graft restricting bending deformation of the host bone and sharing a certain level of mechanical loading, thus reducing the strains and stresses on the plates [375]. Typically, healing period of 3-6 month after the FFF operation can be expected according to our clinical follow-up [408] and modelling study [371]; therefore, it is essential to extend the fatigue life of the fixation plates to ensure the structural reliability during the healing process.

In both the femoral and mandibular reconstruction cases, it can be found that the fixation plates for the segmental defects without bone substitute would have substantially shorter fatigue lifespan. The reason may be attributed to approximation of the loading amplitude and frequency applied. In this study, the loading amplitude was referred to the experimental tests on patients 11-16 months after implantation [375, 385, 411]. In the early healing stage, with the help of crutches and/or wheelchairs, the real load borne by the fixation plate would be substantially lower than the value adopted here. In addition, the loading cycles during the early stage could be much fewer than 5000 per day for the femur fixation plate, and 600 per day for the mandible reconstruction plate [370, 385].

There are many other factors that may have caused inaccuracy in the present fatigue life predictions. While the presented XFEM fatigue analysis can to a certain extent simulate the clinical situations, it is still demanding to consider all the clinical factors more realistically.

For example, the current work adopted a constant loading amplitude for both case studies; whereas some clinical studies had suggested that the loading amplitude and frequency can change over the bone remodelling/healing period [408-410]. Further studies, especially considering loading spectrum along with bone remodelling process of the segmental bone defect [371], would be necessary in order to develop a more genuine time-dependent biomechanical fatigue analysis for the plates.

Despite the abovementioned limitations, the presented XFEM fatigue analysis procedure exhibited considerable potential for orthopaedists and biomedical engineers to generate a quantitative estimation of how long a surgical device could last and when the implant has to be replaced to prevent catastrophic failure. In addition, the predicted fracture patterns could become an important indicator to design of fixation plates for specific patients [371].

6.5 Conclusion

This study aimed to develop an XFEM-based procedure for modelling the fatigue failure process of bone fixation plates subject to cyclic loading. First, a benchmarking engineering problem of a modified compact tension structure was investigated for validation purpose, through which good agreement with the experimental data was obtained. Second, the proposed method was used to predict the fatigue lifespan and cracking path for two common clinical examples that involve different fixation devices for supporting tissue scaffold (namely femoral osteofixation plate) and bone graft (namely mandibular reconstruction plate) treatments. This study divulged the importance of bone healing and tissue ingrowth to the fatigue life of fixation plates, where positive bone remodelling can substantially extend the lifespan of the plates. By comparing the results from the healed bone system with initial

segmental counterparts, the stress level in the plate decreased progressively in the course of treatment when the healed bone becomes more mature and more supportive. In addition, the XFEM results revealed that the screw holes largely contributed on fatigue crack initiation and propagation, which requires further investigation. Overall, this study showcases an effective approach for simulating fatigue behaviour of biostructures, thereby evaluating the potential longevity of a prosthetic system. The predicted fatigue life and crack patterns can be used as a guideline for design of reconstruction devices to ensure durability on a patient specific basis.

Chapter 7: On interaction between fatigue of reconstruction plate and time-dependent bone remodelling

The fibula free flap (FFF) has been extensively used to repair large segmental bone defects in the maxillofacial region. As discussed in the previous chapter, the reconstruction plate plays an important role in maintaining stability and load-sharing while the fibula unites with adjacent bone in the course of healing and bone remodelling. However, not all fibula flaps will fully unite, and fatigue of prosthetic devices has been recognized of major concern for long-term load-bearing application. This study aims to develop a numerical approach for predicting the fatigue life of the reconstruction plate by taking into account the effect of ongoing bone remodelling. The changing mineral density and Young's modulus of bone are predicted in a step-wise fashion based upon Wolff's law, which is correlated with specific clinical follow-up. The effects of masticatory forces measured over time on the fatigue life of fixation plate and bone remodelling are also analyzed. Under various occlusal loadings, the interaction between fatigue crack growth and bone remodelling is investigated to identify new insights for design of prosthetic devices. The simulation results indicate that appropriate remodelling of grafted bone could extend the fatigue life of fixation plates in a positive way. However, the healing associated rising occlusal load could lead to fixation plate fatigue fracture and potentially cause severe bone resorption. This study is believed to be the first of its kind to investigate the coupled effect of fatigue of fixation plate and bone remodelling. It showcases an effective approach for predicting fatigue failure of prosthetic devices *in-silico*.

It is anticipated this approach will guide the optimal design of patient-specific prosthetic devices to ensure their longevity.

7.1 Introduction

Large mandibular defects resulting from trauma, tumor, or osteonecrosis signify some clinical challenges facing clinical treatments. Repair of such major bone defects becomes necessary when a significant amount of bone cannot be regenerated spontaneously. Currently, the fibula free flap (FFF) remains the most common option for mandibular reconstruction, owing to its advantages of adequate bone length, low donor site morbidity, long pedicle length, and an abundant periosteal blood supply [370, 408]. The incorporation of a reconstruction plate plays a key role in not only fixating the fibula segments for healing, but also bearing physiological load induced by daily functionality, thereby maintaining the stability of fixation during the bone healing and remodelling over time [421, 422]. A range of fixation plates made of biocompatible metallic alloys has been widely adopted clinically, among which titanium has become a typical material of choice and been used extensively for mandibular fractures and reconstruction. Nevertheless, complications, such as plate fracture, plate exposure, or screw loosening, are still reported frequently, which considerably compromise long-term success and cause severely unfavourable outcomes of treatments [421, 423].

Clinical evidence and specialized literature show that when titanium reconstruction plates are used to bridge mandibular defects without a properly vascularized bone graft, they can experience excessive mechanical stress, possibly leading to fatigue fracture [375, 423]. Studying the fatigue characteristics of such medical devices is thus fundamental and critical,

particularly for load-bearing prostheses, which play an important role in restoring physiological functions with sufficient longevity [424, 425]. Many attempts have been made to characterize the fatigue crack propagation in prosthetic implants experimentally. Digital image correlation (DIC) is one of the most commonly used techniques due to its non-contact nature and measurement features. It can directly provide full-field displacements and strains to sub-pixel accuracy by comparing the digital images of a test object surface acquired before and after deformation [426]. In this regard, Yang et al. quantified the fatigue strength and extent of prosthesis loosening by using DIC [231]. Shen et al. [426] described a new test approach to evaluating the performance of foot implant devices with the help of in-situ 3D-DIC measurements. More recently, Shen et al. [427] also proposed a locking implant and found that its strain can be distributed more effectively under the cyclic loadings through the DIC measurement, thereby reducing the fracture risks.

Various numerical techniques represented by finite element method (FEM) have been extensively utilized for predicting the fatigue life of prosthetic devices [296, 428, 429]. For example, Merema et al. developed a finite element (FE) based design approach for reducing the risk of fatigue failure of load-bearing fixation plates by designing a novel titanium bridging prosthesis [430]. Hung et al. investigated the fatigue failure of cemented hip prosthesis through the numerical approaches [50]. Villa et al. estimated the fatigue failure risk of total knee prosthesis on the basis of FE modelling [431].

Based upon linear elastic fracture mechanics (LEFM) theory, numerical methods have also been developed to mimic the cracking path and estimate fatigue life of structure [432]. LEFM (originated by Griffith and enhanced by Irwin) provides a theoretical framework for predicting fatigue crack growth in various engineering problems, which constitutes a basic

fracture mechanics theory for characterizing stress fields in the vicinity of a crack tip [387, 432]. Based upon LEFM, Jones and Dunn used FE analysis to compute stress intensity factors in crack tip, thereby estimating crack growth; and their simulation results were validated through the experimental data obtained from single-edge bend specimens made of 2024-T351 aluminium alloy [433, 434].

To analyze 3D crack propagation in relatively complex geometries, adaptive FE remeshing techniques have been widely adopted in literature [435]. For example, Zhang et al. conducted a numerical study on fatigue crack growth in a gear tooth by using FRANC3D [436]. Schöllmann et al. developed a new fatigue crack growth algorithm to simulate crack propagation in knee-levers by using two commercial programs, FRANC/FAM and ADAPCRACK3D [437]. In spite of its predictive functions, the limitation associated with this type of numerical approach resides in the time-consuming and inadequate simulation accuracy due to frequent changes in mesh topology in the course of crack tip extension.

To overcome the abovementioned numerical difficulties, the eXtended Finite Element Method (XFEM) provides a relatively newer approach to simulation of crack propagation without constantly re-meshing the FE model; as a result, the crack location and geometry can be more easily determined without altering the initial mesh. Recently, some studies have employed XFEM framework to model fatigue crack growth in several engineering applications. For example, Bergara et al. evaluated the fatigue crack propagation in complex stress fields using XFEM [387]. Dirik and Yalcinkaya adopted XFEM to estimate the crack path of a polymethyl methacrylate (PMMA) beam under mixed-mode cyclic variable amplitude loading [391].

Our previous work investigated the structural stability and integrity of the reconstruction plate, which however had not considered the ongoing effects of bone remodelling; thereby the prediction of fatigue life was therefore effective only for several specific time points after implantation [424]. When a reconstruction plate is placed in a patient's body, the surrounding host bone and bone graft continuously remodel themselves to adapt to the new biomechanical environment; thus, the overall stiffness of the prosthetic system would continually change over time [371]. On the other hand, crack initiation and propagation induced by excessive loads will also affect the stiffness of the plate and, in turn, the associated bone remodelling by varying the mechanical loading transferred onto the bone. Note that from a biomechanics point of view, bone remodelling signifies a biological process in which bone constantly evolves its density and adapts its morphology to accommodate variation in a specific mechanobiological environment. Wolff's early study introduced this concept by relating bony structure to mechanical loading [438]. Since the establishment of Wolff's law, numerous theoretical and computational approaches have been proposed to simulate and predict bone remodelling processes [439-442]. Nevertheless, it remains demanding to perform a coupled analysis considering the interaction between bone's ongoing remodelling and prosthetic fatigue characteristics.

This study thus aims to develop a novel computational approach for investigating the coupling effect between bone remodelling and fatigue behaviour of mandibular reconstruction plates, thereby gaining a better understanding of their interactive influence on long-term therapeutic outcomes. In this work, a time-dependent XFEM fatigue analysis associated with a time-dependent bone remodelling simulation is coupled in a step-wise fashion. Accordingly, the biomechanical and fatigue responses, such as mechanical stimulus, bone densities, stress states, and resultant crack patterns, are analyzed in detail. The

simulation results indicate that the remodelling of grafted bone would have a significant bearing on the fatigue life of fixation plates, and vice versa. This study showcases an effective approach for realistically predicting fatigue failure of prosthetic devices within a varying biomechanical environment *in-silico*. Such a strategy is anticipated to provide clinical guidance for design optimization of patient-specific prosthetic devices to better ensure their longevity.

7.2 Materials and methods

7.2.1 Fatigue damage modeling

In the proposed numerical analysis, the direct cyclic algorithm (Abaqus/Standard) is used to model the low cycle fatigue (LCF) behaviour of a mandibular reconstruction plate. Based on a continuum damage mechanics framework, the direct cyclic algorithm provides a computationally effective modelling approach for obtaining the stabilized response of a structure subjected to cyclic loading [136]. In the computational analysis, the LCF process is modelled as per progressive damage and cracking failure. The mechanical responses are identified by evaluating the structural behaviour along with a specific loading history. The obtained results are then used to predict the evolution of stiffness due to degradation of the material properties, which are updated iteratively and considered in the subsequent calculation step. The degraded material properties of the construction plate are then used to determine the new solution at the next incremental time point over the loading history [392]. Therefore, the damage evolution rate is updated in each increment continually throughout the iterative analysis [424].

The crack initiation criterion is based upon the stabilized accumulating hysteresis strain energy per cycle, ΔW , which can be expressed mathematically as [139, 396],

$$N_0 = A(\Delta W)^B \quad (7.1)$$

where N_0 is the number of cycles towards damage initiation, ΔW is the hysteresis strain energy per cycle, A and B are material constants, which can be determined via a fitting exercise to correlate with the corresponding LCF-experimental data. In this study, a value of $5.17 \times 10^5 (mJ/mm^3)^{-B}$ for parameter A and a value of -2.37 for parameter B were used for the titanium alloy concerned [443, 444].

Once the crack has initiated, the maximum principal stress criterion is employed to determine the crack growth direction [392]. A crack evolution model is employed to simulate the degradation of material stiffness after damage initiation [392]. In the computational analysis, the damage accumulation is characterized by the stress intensity factor (SIF) (K) at the crack tip in line with the Paris law [392, 393]. The range of SIF (ΔK) under cyclic loading with a constant amplitude can be calculated as,

$$\Delta K = K_{max} - K_{min} \quad (7.2)$$

where K_{max} and K_{min} are the stress intensity factors corresponding to the maximum and minimum loads applied, respectively. The generalized Paris law can be expressed as [413],

$$\frac{da}{dN} = C(\Delta K)^n \quad (7.3)$$

where a is the crack length (the original crack length is associated with the local FE mesh that is approximately 0.047 mm here), and N the number of loading cycles. C and n are

material dependent constants, which are taken as $5.88 \times 10^{-8} \text{ (mm/cycle)}$ · $\left((MPa\sqrt{m})\right)^{-n}$ and 3.17 for the titanium alloy, respectively [444].

The Paris regime is bounded by the threshold SIF (K_{th}) and fatigue critical SIF (K_{fc}) values [391]. When ΔK is lower than K_{th} , the crack will not propagate; whilst once ΔK exceeds the K_{fc} value, the fatigue crack grows at an accelerated rate, which generally leads to unstable cracking. Note that in a region of stable fatigue crack propagation, the crack growth rate (da/dN) is dependent upon the SIF [381]. At the time of failure, the number of cycles elapsed can be determined, thus providing an estimation of the fatigue life of the structure.

Further, the stress intensity factor was also used to measure crack growth for mixed-mode fatigue, which can be calculated based upon a user-specified criterion. This study follows Nikfam et al. in terms of a joint SIF, specifically [388],

$$\Delta K_{eq} = \sqrt{\Delta K_I^2 + \Delta K_{II}^2 + \Delta K_{III}^2 / (1 - \nu)} \quad (7.4)$$

where K_I , K_{II} , and K_{III} represent the SIFs in fracture modes I, II and III, respectively, and ν is the Poisson's ratio of the material.

7.2.2 eXtended finite element method (XFEM)

In the present study, fatigue cracks are simulated in XFEM by introducing phantom nodes to the existing elements which involve the crack discontinuity, as the additional degrees of freedom enable an enrichment of the finite element approximation. To describe the mathematical background of XFEM, let all the nodes involved be denoted by set D , and the nodes around the cracking surface and tip are represented by the subset D_s and D_t ,

respectively. Thus, the approach for displacement calculation with crack modeling in XFEM has a form given in Eq. (6.5) [413],

$$\mathbf{u}_{XFEM} = \sum_{i \in D} N_i(x)(\mathbf{u}_i) + \sum_{i \in D_s} N_i(x)H(x)(\mathbf{a}_i) + \sum_{i \in D_t} \left[N_i(x) \sum_{\alpha=1}^{ne(j)} F_{\alpha}(x)(\mathbf{b}_i^{\alpha}) \right] \quad (7.5)$$

where $\mathbf{u}_{XFEM}$ is the enriched displacement vector, N_i is the standard nodal shape function, $\mathbf{u}_i$ stands for the nodal displacement vector for non-enriched nodes, $H(x)$ denotes the Heaviside function, $\mathbf{a}_i$ is the enriched nodal degree of freedom vector associated with the Heaviside function. $F_{\alpha}(x)$ represents asymptotic crack tip function, $\mathbf{b}_i^{\alpha}$ stands for the nodal enriched degree of freedom vector associated with crack tip enrichment.

7.2.3 Bone remodeling algorithm

The FE-based bone remodeling prediction requires quantifying the biomechanical responses of site-dependent units (e.g., elements) within the bone subject to mechanical loads. Once the mechanical stimulus deviates to a certain extent from the specific homeostatic level, the bone will respond by adapting its morphology to such a change. In the literature, a scalar quantity, strain energy density (SED) per unit density, has been widely accepted as an appropriate mechanical stimulus for bone remodeling [408, 440, 445], which is defined by

$$\mathcal{E} = \frac{U}{\rho} \quad (7.6)$$

where U , ρ , and $\mathcal{E}$ are the SED (J/cm^3), local bone density (g/cm^3), and mechanical stimulus (J/g), respectively. The remodeling response and bone density can thus be determined in terms of the mechanical stimulus and its physiological threshold Θ . Specifically, the density increment ($\Delta\rho$) over a time interval (Δt) can be evaluated as,

$$\Delta\rho = \begin{cases} C_{ap}[\mathcal{E} - \Theta(1+s)]\Delta t - C_{or}[\mathcal{E} - \Theta(1+s)]^2\Delta t; & \text{if } \mathcal{E} > \Theta(1+s) \\ 0; & \text{if } \Theta(1-s) \leq \mathcal{E} \leq \Theta(1+s) \\ C_{ur}[\mathcal{E} - \Theta(1-s)]\Delta t; & \text{if } \mathcal{E} < \Theta(1-s) \end{cases} \quad (7.7)$$

where the reference stimulus $\Theta = 0.00036 \text{ (J/g)}$ and $2s = 0.2$ is the width of the lazy zone [371, 408]. C_{ap} , C_{or} , and C_{ur} are the rate constants ($C_{ap} = C_{ur} = 18 \text{ (g/cm}^3\text{)}^2\text{/J/month}$, $C_{or} = 600 \text{ (g/cm}^3\text{)}^3\text{/J}^2\text{/month}$) for bone apposition, overloading resorption and underloading resorption, respectively.

As previously reported in literature, the rate of change in bone density with respect to the mechanical stimulus includes three phases, namely underloading bone resorption, bone equilibrium (or so-called lazy zone), and bone apposition [371, 439]. It should be noted that the bone density cannot keep rising indefinitely with an increase in mechanical stimulus as damage can be caused if the loading is excessively higher than a critical value for physiological self-repair in the bone. Therefore, to consider bone resorption induced by overloading, a quadratic term was introduced to the bone apposition phase in Eq. (7.7) once the mechanical stimulus exceeds the physiological limit [446].

After the density is determined via the remodeling calculation in Eq. (7.7), the Young's modulus of the bone can be updated by its varying density, an empirical formula of which is defined as [371, 408],

$$E_i = \alpha \rho_i^\beta \quad (7.8)$$

where E_i is the Young's modulus after i month remodeling. α and β are material constant and material exponent, respectively. In this study, a value of $1895 \text{ MPa} \cdot (\text{g/cm}^3)^{-\beta}$ for parameter α and a value of 3 for parameter β are used through the clinical correlation [371].

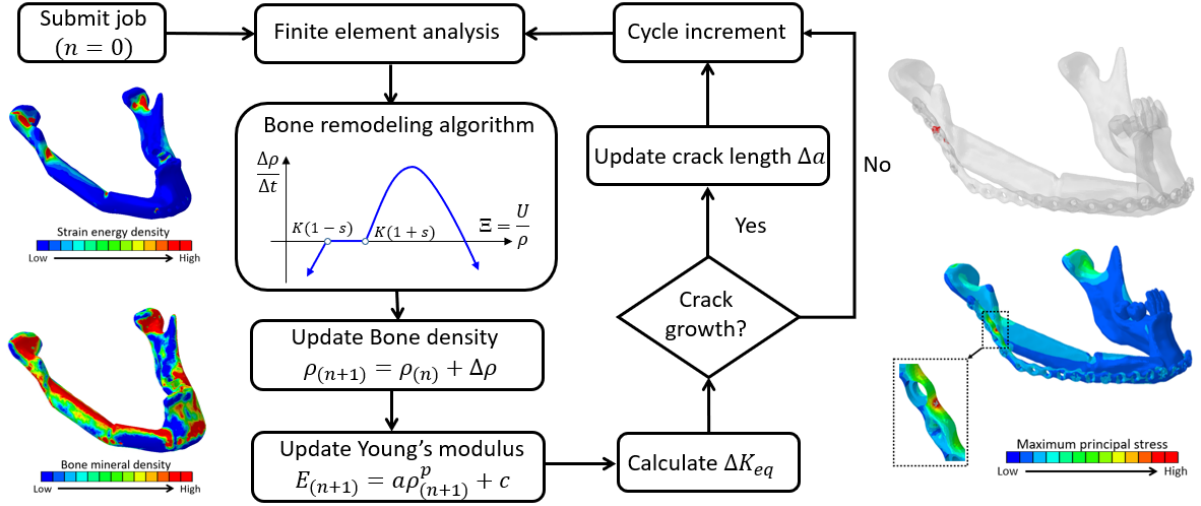


Figure 7.1: Flowchart for integrating the XFEM based fatigue crack growth with time-dependent bone remodeling.

The remodeling procedure is implemented in Abaqus through a FORTRAN subroutine (UMAT), where the material properties of bone in each element were evaluated as per the user-defined constitutive models. A flowchart is provided in **Figure 7.1** to depict the numerical procedure by coupling the time-dependent fatigue cracking analysis with time-dependent bone remodeling simulation. In the proposed coupled procedure, the FE analysis is first performed to obtain the mechanical stimulus (SED) in the bone. By using the bone remodeling algorithm, the change in bone density is predicted in a step-wise manner as in Eq. (7.7). Following the update of Young's modulus of the bone in Eq. (7.8), the equivalent SIF of the prosthetic plate is calculated based upon Eq. (7.2). With XFEM, the increments in cracking size during loading cycles are updated by using the Paris law as in Eq. (7.3). The above steps are repeated until the equivalent SIF exceeds the fracture toughness of the plate material or the predetermined remodeling time period is achieved (40 months here).

7.2.4 Clinical measurement of biting force

In this study, the biting force (mastication) is considered as the functional load driving the bone remodeling and fatigue of the titanium fixation plate. To consider the effects of mastication, the maximum biting forces on remaining teeth are measured clinically at different time points at 4 (M4), 16 (M16) and 28 (M28) months after reconstruction surgery, respectively. Pressure-indicating film (Dental Prescale 50H, type R, Fuji Photo Film Co., Tokyo, Japan) and a pre-calibrated device (Occluzer FPD 707, Fuji Photo Film Co.) was used to measure the biting forces. It is seen that the maximum biting force gradually increases with time (M4, M16, M28) after surgery. As a result, three loading cases which take into account different biting force levels are studied here, as detailed in **Table 7.1**.

Table 7.1: Details of the upper limit of biting force measured at different time points after reconstruction surgery (Unit: N)

Month		0	4	16	28	40 (end)
Load Case-A	Muscle force		46	56	82	-
Load Case-B	Muscle force		58	85	116	-
Load Case-C	Muscle force		91	105	165	-

7.2.5 Clinical data and finite element models

In this study, longitudinal CT data was obtained clinically from a specific patient who underwent mandibular reconstruction with an osteotomized fibular free flap due to a

squamous-cell carcinoma of the right lower gingiva. A stock titanium fixation plate (Synthes, Solothurn, Switzerland) was pre-bent using the CT-based 3D patient model prior to the surgery, and attached monocratically with a total of 11 titanium screws (Synthes, Solothurn, Switzerland). The follow-up CT images were taken at 4, 16, 28 and 40 months after surgery (namely, M4, M16, M28, and M40, respectively) [408].

The longitudinal CT images were imported into ScanIP Ver. 4.3 (Simpleware Ltd, Exeter, UK) for segmentation. The segmented masks, including bone, individual teeth and periodontal ligaments (PDL), fixation plate and screws, were further processed in Rhinoceros 4.0 (Robert McNeel & Associates, Seattle, USA) to create parametric models with non-uniform rational B-spline (NURBS). Finally, the geometric models were imported into commercial FE code Abaqus (ABAQUS, Inc, Providence, RI). The mandible, fibular bone, teeth, screws, and plate were meshed using the 4-node linear tetrahedral elements in Abaqus. A mesh convergence test was conducted to balance the computational cost and numerical accuracy, and the total number of elements in the FE model was 749,408 with 424,227 degrees of freedom.

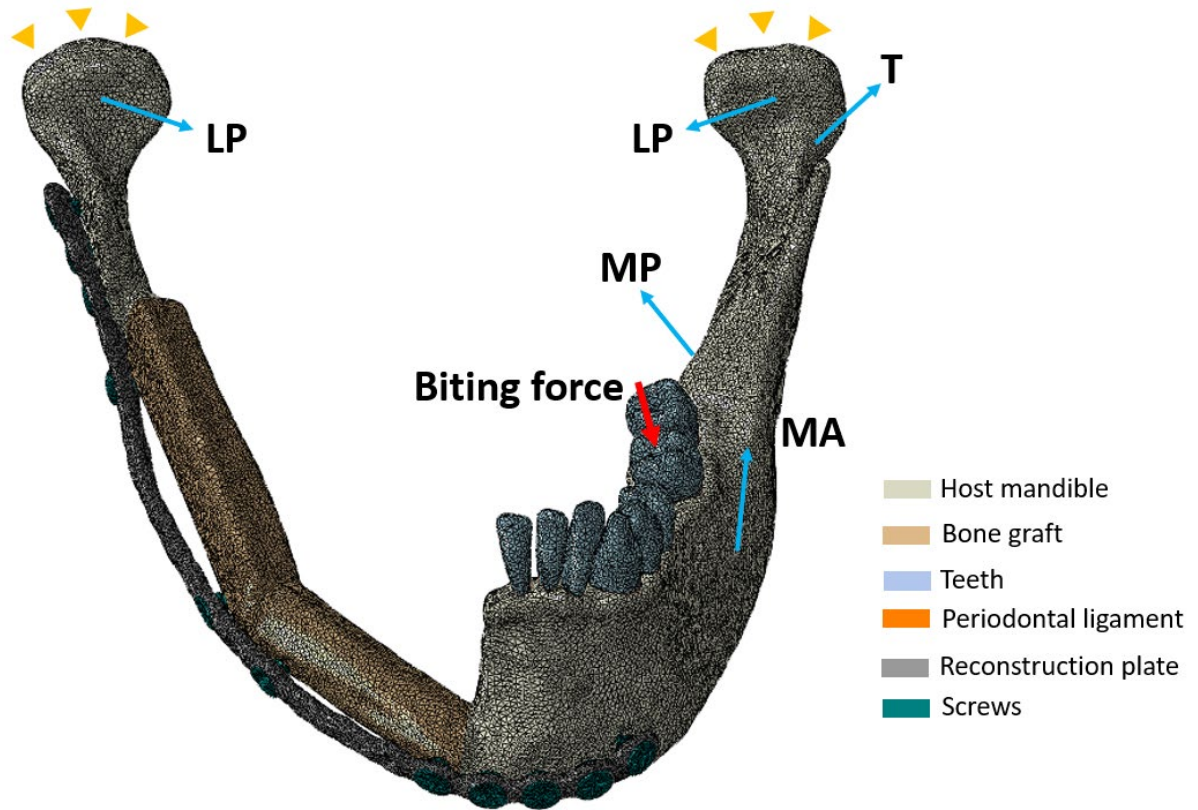


Figure 7.2: 3D CT-based FE model with a reconstruction fixation plate, screws, fibula free flap, and its loading/boundary conditions. The blue arrows indicate muscle forces, e.g., Lateral pterygoid (LP), temporalis (T), medial pterygoid (MP), and masseter (MA). Yellow triangles show the kinematic constraints around the temporomandibular joints.

The loading and boundary conditions of the mandibular model are described in **Figure 7.2**. The muscular forces, including masseter (MA), medial pterygoid (MP), lateral pterygoid (LP), and temporalis (T) muscle, are applied to simulate the muscle forces during the bone healing period (M1 – M4) [408]. The magnitudes and directions of muscle forces are derived based upon the clinical data: MA as 59.23 N, MP: 39.60 N, LP: 34.44 N, and T: 34.09 N, respectively [410].

According to the literature, a cyclic biting force is applied on the left second molar (30° buccolingual inclination to the normal axis of the occlusal surface of the second molar) [411]. The lower limit of the biting forces is considered to be a constant (0 N), and the upper limits are the maximum bite forces measured at different time points clinically (M4, M16 and M28), as summarized in **Table 7.1** [421, 447]. The temporomandibular joints are assumed to be fully constrained, and the interfaces between the plate and screws, as well as the interface between the screws and the mandible bone, are considered to be fully bonded after a certain period of osseointegration [370, 375].

In this study, the mandibular bone and fibula graft are approximated to be heterogeneous, bone density-dependent isotropic and linear elastic materials to more realistically mimic the biomechanical response [86, 412]. A voxel-based mapping algorithm was implemented in this study to calculate the heterogeneous density distribution of the reconstructed mandible based upon the localized Hounsfield Unit. The corresponding Young's modulus can be further estimated from the CT-based bone density. The surgical reconstruction plate and screws are made of titanium ASTM F67/2 (Ti grade 2), which is considered isotropic and linear elastic in the fatigue analysis [448]. The mechanical properties of all the materials used in the numerical simulations are summarized in **Table 7.2**.

Table 7.2: Material properties of the simulated mandible and reconstruction plate system [424] [395].

Materials	Young's Modulus E (MPa)	Poisson's Ratio ν	Yield Strength σ_Y (MPa)	Ultimate Tensile Stress σ_{TS} (MPa)	Fracture Toughness K_{IC} (MPa·m ^{1/2})
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Plate	105×10^3	0.3	276	445	29
Screw	105×10^3	0.3	276	445	29
Mandible	Heterogeneous	0.3	-	-	-
Fibula	Heterogeneous	0.3	-	-	-
Tooth	80×10^3	0.28	-	-	-
PDL	70	0.45	-	-	-

7.3 Results

In this section, the fatigue behaviors and the interactions with the bone remodeling process of a typical mandibular reconstruction plate used to fixate a fibula free flap for proper reconstruction of segmental mandibular defect are studied.

The maximum principal stress (MPS) was calculated (**Figure 7.3**) in the reconstructed mandibular system with various occlusal loadings. It can be seen that in general, the stress magnitude in the mandible was substantially lower than those in the screws and plate; and the region with the highest stress values occurred in the reconstruction plate. According to **Figure 7.3(a)-(c)**, it is evident that load Case-A had a more even stress distribution in the entire plate compared with the other two. In Cases-B and C, the stresses were mainly concentrated on the curved inner side of the plate and further at the notch of the plate edge. As expected, the comparison indicates that more extensive occlusal loading leads to a higher stress concentration in the plate. For different loading cases, Case-C presented the highest peak stress value (355.55 MPa), followed by Case-B (301.78 MPa) and Case-A (220.59 MPa).

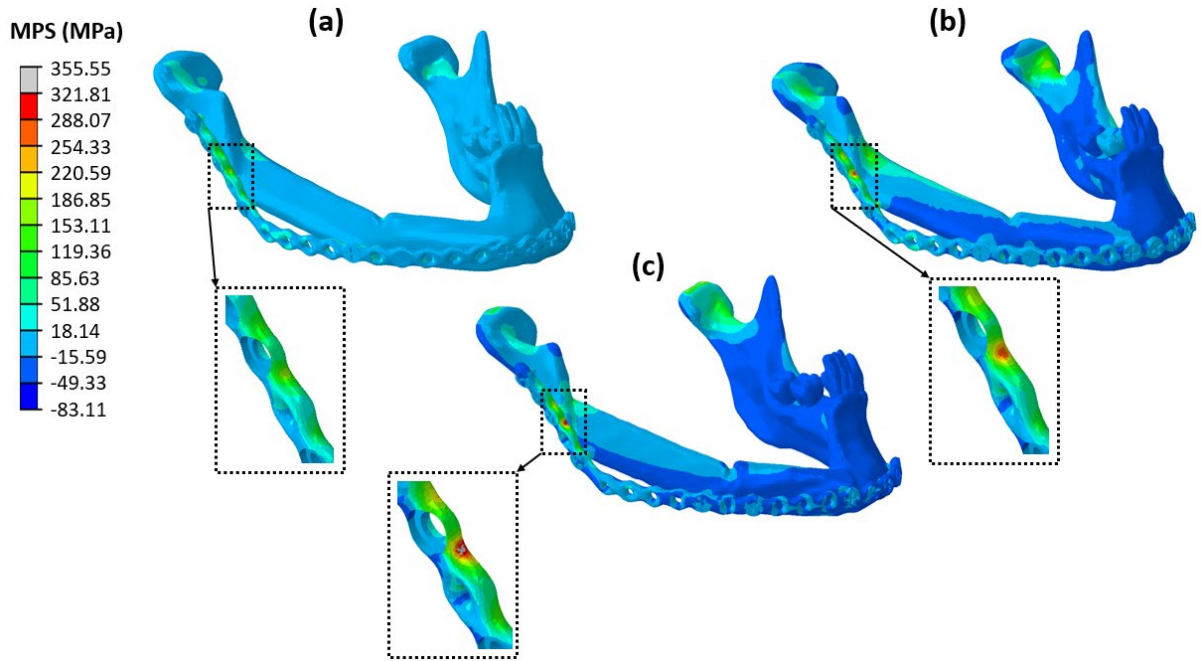


Figure 7.3: The maximum principal stress (MPS) distribution in the mandible and reconstruction system for different load cases. (a) Case-A. (b) Case-B. (c) Case-C.

The representative crack origin site and propagation path (as exemplified from Case-C) are depicted in **Figure 7.4(a1)**. According to our previous study, the summation of continuous chewing time was approximated to be 10 minutes during a day at a chewing rate of 60 cycles per minute [424]. This is equivalent to 600 cycles per day and approximately 1.8×10^4 cycles per month. In line with this estimation, the fatigue life of the reconstruction plate can be presented in a unit of months.

For the load Case-C shown in **Figure 7.4(a2)**, the crack is found to originate at month 4 and propagated during the following treatment period until month 32 when the plate was fully cracked. It can also be seen that multiple cracks initiated from the thinner regions around the

plate holes (**Figure 7.4(a2 - i)**). Note that while multiple cracks were initiated almost simultaneously, only one crack propagated extensively as the loading cycles increased, which is named a primary crack. The primary crack propagation was found in the plate and nucleated at the notch of the plate near the distal side of the bone graft margin, which is the stress concentration site (**Figure 7.4(a2 - ii)**). **Figure 7.4(a2 ii–v)** show the crack propagation path that develops across the entire thickness of the plate, and ultimately the plate completely fractured (**Figure 7.4(a2 - v)**).

Figure 7.4(b) shows a radiographic image of fracture of a titanium reconstruction plate in the early stage following the FFF-based reconstruction surgery. It can be observed that although there are some modelling discrepancies to the real surgical operation, the simulated rupture pattern (**Figure 7.4(a1)**) exhibited fairly good correlation with the clinical observation, specifically the fracture occurred near the distal side of the reconstructed mandible.

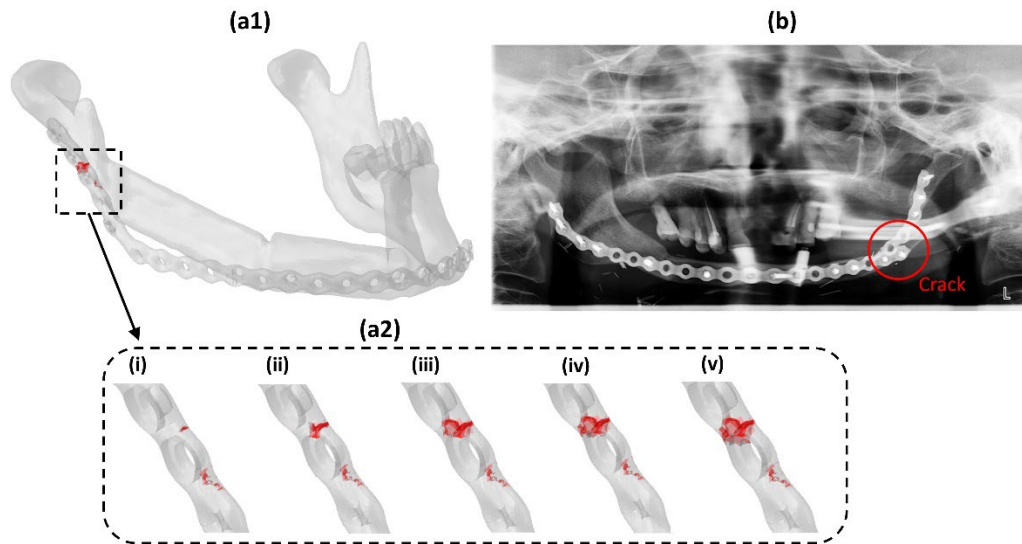


Figure 7.4: (a1) The simulated crack pattern in the reconstructed mandible. (a2) The crack propagation path at different time points for a representative loading case (Case-C); (i) 4

month (M4); (ii) 16 month (M16); (iii) 28 month (M24); (iv) 30 month; (v) 32 month. (b) Radiographs of a fractured reconstruction plate (22 months after the reconstruction surgery).

Figure 7.5 compares the distribution of the apparent bone density in the reconstructed mandible under these three loading scenarios after 4 months and 32 months post-surgery. To understand the effect of plate fatigue fracture on the bone remodeling process, we would focus on the posterior fibula graft where the crack took place in the fixation plate, shown as the cross-sectional view in **Figure 7.5**. At the initial stage of bone remodeling, the distribution of apparent density in the overall fibula graft and the cross-sectional view appears similar in all the loading cases. In general, the simulated density increased faster in the upper region of the fibula graft in comparison with the other areas, implying a high level of mechanical stimulus accumulated there. Furthermore, from the sectional view of the mandible, the remodeling activity in the central area of the mandible appeared less vigorous than the peripheral region. In Case-B, the bone density contour at month 32 showed a marginal decrease at the posterior end of the fibula graft; whereas Case-C exhibited a significant density loss in a similar region compared to Case-B. According to the sectional view, the decrease in bone density occurred from the peripheral region first, then propagated to the center of fibula graft.

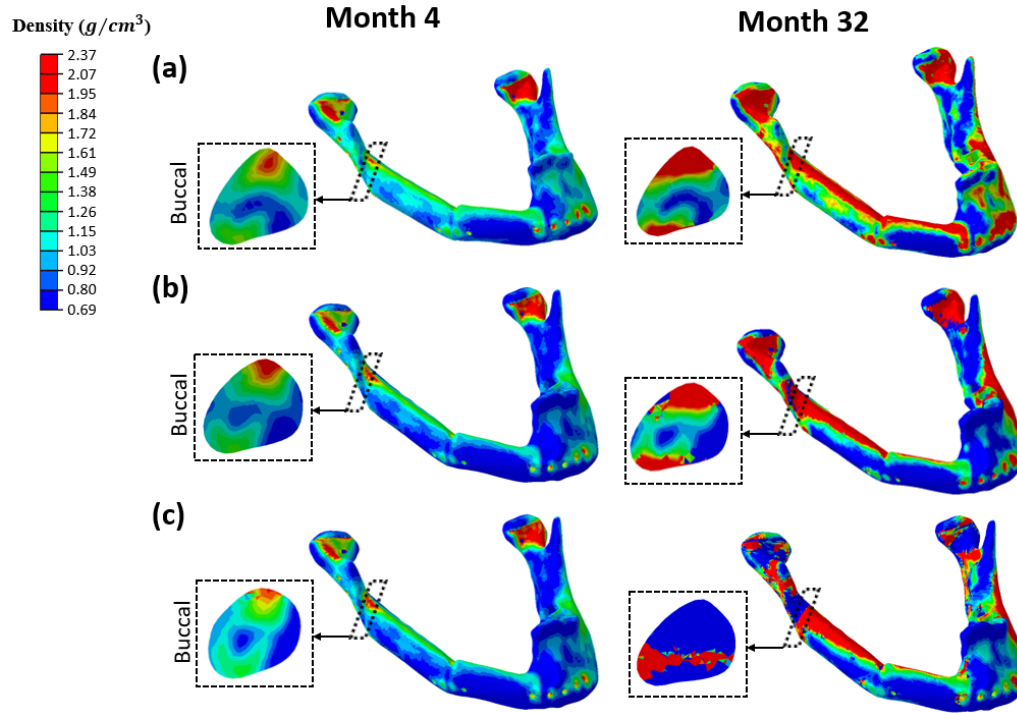


Figure 7.5: The apparent bone density distribution for the models under the three different loading scenarios. Bone density distribution was shown at two different time points (4 months and 32 months) after surgery, and the cross-sectional view of the posterior end of the fibula graft where the crack occurred in the plate. (a) Case-A; (b) Case-B; (c) Case-C.

Figure 7.6 depicts the bone mineral density development near the cracking site of the reconstruction plate. To calculate the average bone density of the fibula graft near the cracking site, a 10 mm^3 volume of interest (VOI) was selected from the posterior end of the fibula graft. It is seen that the magnitude of average bone density of the VOI gradually increased in Case-A, especially from months 0 to 12. The bone remodeling appeared to stabilize after month 12, and the mean value in the bone graft is close to 1.39 g/cm^3 . For Case-B and Case-C, while a minor decrease in density can be observed from month 4 to month 9, the density continuously increased during the subsequent period. Remarkably, the slope of density increase became steeper at month 16, which signifies a higher bone growth

rate. After that, the bone density with Case-B experienced a marginal drop at month 28 then approached an equilibrium state, where the bone density was 1.33 g/cm^3 . Nevertheless, a substantial drop in density can be found in Case-C at month 28 and ends at month 32 when the plate was fully fractured.

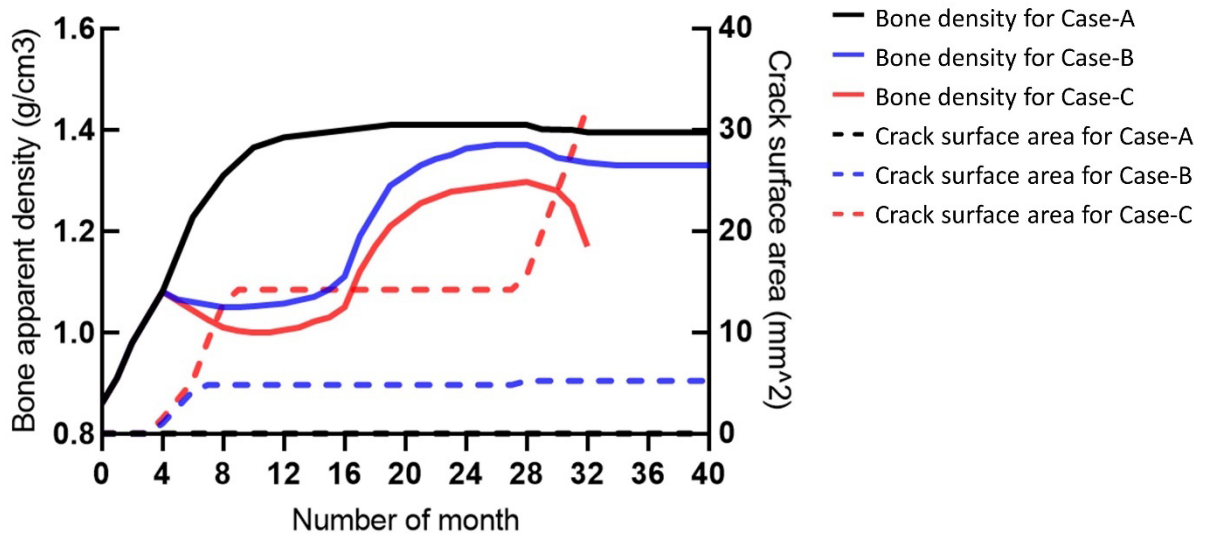


Figure 7.6: The evolution of bone mineral density (left Y-axis) and crack surface area (right Y-axis) for three loading case scenarios over the 40 months of the remodeling period.

According to the cracking area presented in **Figure 7.6**, there was no crack in the fixation plate under load Case-A; therefore, the corresponding crack surface area stayed at 0 over the entire remodelling period. In Cases B and C, on the other hand, the cracks both initiated at month 4 and then propagated at different rates. Specifically, the crack of Case-C grew considerably quicker than Case-B, e.g., at month 8, the crack surface area in Case-C (12.8 mm^2) was more than twice of Case-B (4.8 mm^2). Interestingly, a plateau in the crack area can be found after month 9 for both Cases B and C, implying that the crack may have somehow been arrested. Following the plateau, there was a significant increase in the

cracking area during months 28-32. At this stage, the final fracture can be seen in the plate at month 32, and the corresponding crack pattern is shown in **Figure 7.4(a2 - v)**. In Case-B, the crack was fairly stable since it was arrested at month 9, while there was a minor increase at month 28 but remained stable thereafter.

7.4 Discussion

Most previous studies on fatigue life of fixation plates have commonly adopted a fatigue strength curve, also known as an S-N curve, which relates the number of cycles or fatigue life (N_f) with stress amplitude (σ_a) [375, 430, 449]. For example, Hoefert and Taier evaluated the fatigue life of commercial mandibular bridging plates and optimized the stress on the plate to reduce the incidence of plate fractures [375]. They identified that the most problematic regions with high stress concentrations are the inner curvature of the plate and the notch of the plate edge, which is similar to our observation as shown in **Figure 7.3**. However, the conventional S-N curve cannot present the real crack pattern and propagation path in the plate. This inability to reveal the relationship between the cracking process and loading cycles makes prediction of its ongoing interaction with bone remodeling difficult. The presented XFEM based simulations suggest that the cracking site is closely related to the area with a higher MPS magnitude, which is supported by literature describing that stress levels above the fatigue endurance limit would lead to failure of plate over time [450, 451].

Not only did the identified crack origin site and propagation path in **Figure 7.4** show reasonable agreement with the clinical observation, but also corresponded to the common areas where cracks developed in structurally failed plates reported in literature [423]. The maximum biting force resulted in the inner curvature of the plate being more vulnerable to

crack initiation [450, 452]. Because of the specific geometry of the plate, a stress concentration develops in the notch of its inner curved surface. Martola et al. [423] calculated the stress concentration factor for the notch region and found that the factor varied between 1.27 and 1.51, with an average of 1.39. This means that the stress around the notch was 1.39 times the average stress in the reconstruction plate under the maximum biting force.

Mechanical loading within the physiological limit is known to be beneficial for proper bone healing and remodeling, likely enhancing bone mass and strengthening its functionality over time [440, 453, 454]. In other words, mechanical stimulus plays an important role in affecting bone remodeling activity. During functional loading, the maximum stress in the plate is observed in the region which is near the posterior end of the fibula graft (**Figure 7.3**). Accordingly, the overall mechanical stimulus (e.g., strain energy density in this study) reaches a maximum value in the symphysis region. A high SED leads to bone growth taking place quickly in this region. According to the simulated bone density contour at month 4 seen in **Figure 7.5**, the primary bone density increase is observed to occur more in the superior region of the fibula graft.

Considering the steady increase in the bone density as a result of bone apposition in the fibula graft over the first 16 months (**Figure 7.6**), the bone graft established a better strength and higher stiffness to gradually accommodate a rising occlusal load [440]. Accordingly, there is no plate crack observed in Case-A as shown in **Figure 7.6**. Therefore, under moderate occlusal loading, bone remodeling activity has a primary influence on functional restoration, which plays a role in preventing fatigue cracking. Nevertheless, some studies have shown that after a certain number of month post-surgery, the mechanical stimulus decreased in the graft bone and led to underloading bone resorption [375, 408]. In our present

study, the increase in biting force at months 16 and 28 measured from clinical follow-up could to a certain extent alleviate the reduction in mechanical stimulus and make it be fallen in the lazy zone rather than below the lower thresholds for underloading resorption in the effective SED. This enables to progressively approach towards an equilibrium status of bone apposition, as shown in **Figure 7.5(a)**.

In this study, the different loading amplitudes were referred to our in-house clinical measurements taken at several specific time points (M4, M16 and M28) post-surgery. In general, the increase in the maximum biting force results in a greater mechanical stimulus in the reconstructed mandible. As the mechanical stimulus is considered to be a trigger for bone remodeling, a higher level of SED accumulation leads to a higher rate of bone formation. This may explain the higher rate of bone density increase at month 16 in Cases B and C.

Concerning Case-B, the posterior end of the fibula graft appeared to experience marginal bone resorption once the plate partially failed as seen in **Figure 7.5(b)**. This is due to the fact that the cracked plate cannot bear adequate functional loading; thus, the mechanical stimulus in the VOI exceeded the physiological limit, leading to overloading bone resorption. Regarding Case-C, although there was bone apposition in the grafted bone to some degree over months 0-28, it experienced more significant resorption during months 28-32, as shown in **Figure 7.5(c)**. This is because when the fixation plate fully fractured at month 28, the functional load was transferred from the fixation plate to the fibula graft entirely, thereby causing considerable overloading resorption.

In terms of the fatigue life, the lifespan of the plate in Case-A approaches infinity as no crack was simulated. Although the plate implanted for Case-B partially failed at month 8, the crack appeared to be arrested over the following treatment duration, indicating that the

surrounding bony tissue was able to take up a greater proportion of functional loading. Therefore, the fatigue lifespan of the fixation plate under this loading scenario can also approach infinity theoretically. It must be pointed out, nevertheless, that due to plate imperfections, structural failure may occur as a result of subsequent overloading nearby. Finally, Case-C has a limited fatigue life (32 months) under the relatively higher functional loading, which is consistent with the fatigue life observed clinically [370]. According to work on the plate fractures by Almansoori et al. [376], 54.4% occurred within the first 24 months and 15.1% in the subsequent 12 months, which shows reasonable agreement with the simulated fatigue life of reconstruction plate in our study.

To further elaborate the effect of bone remodeling on the fatigue life of the construction plate, the fatigue crack propagation was evaluated in the same loading cases but without considering the bone remodeling effect. The reconstructed mandible with FFF at the initial stage was considered for comparison, and the corresponding FE model is shown in **Figure 7.7(a)**. A soft-tissue layer (thickness of 0.5 mm) was added in the gap between the host mandible and fibula bone graft to simulate the fibrous tissue during the bone healing state [455]. Idealized isotropic values of Young's modulus and Poisson's ratio for the fibrous tissue were chosen as 200 MPa and 0.4, respectively [385, 424]. According to **Figure 7.7(b)**, it can be seen that the mild occlusal load led to a more gradual tendency of crack propagation.

As reported previously, there was no final fracture observed in either Case-A and Case-B when considering bone remodeling; however, Case-A and Case-B without bone remodeling experienced full plate fracture at M37 and M26, respectively. Regarding Case-C without bone remodeling, due to excessive biting force at M4, it can be found that the crack grew continuously until final fracture at month 11 even without experiencing a plateau. The results

clearly suggest that bone remodeling has a significantly positive effect on extending the fatigue lifespan of fixation plates under various loading conditions. This is due to the fact that bone apposition increases the strength and stiffness of the bone graft, enabling it to support a greater portion of the functional loading.

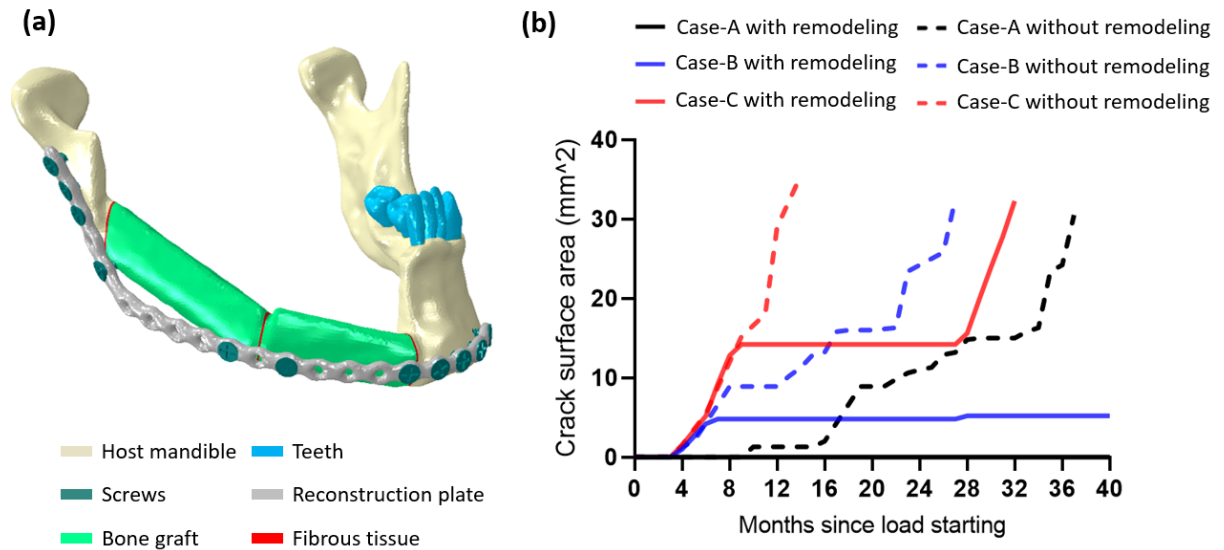


Figure 7.7: (a) FE model of the reconstructed mandible with FFF at the initial healing stage. (b) The development of crack surface area for the mandible models with/without bone remodeling under three loading case scenarios.

However, some simplifications and limitations of this study need to be mentioned. First, the amplitude of the muscle force may change over the bone remodelling period; and the variation in the muscle forces may not only determine the remodelling outcomes, but also affect crack onset location and propagation in the plate [447]. Whereas our study considered only three time points (M4, M16 and M28) measured from clinical follow-up data. In other words, the loading was assumed to be a constant within each measurement duration (M4-M16 and M16-M28) in the remodelling and fatigue simulation.

Second, the current work assumes that the mechanical properties of bone are directly related to bone density without considering a more detailed mineralization process on the microscopic scale. Under this assumption, the effect of bone microstructural variations could not be included in this study. In fact, it is well recognized that the basic unit of mature human cortical bone is the Haversian system or secondary osteon [456-458]. Some researchers stated that Haversian systems under remodelling have a lower degree of mineralization and contain collagen fibrils that are organized into lamellae [456, 457]. Although the proposed study developed a pixel-based mapping algorithm to reconstruct the heterogeneous Young's moduli at different time points, more mechanical gradients in the bony tissue need to be considered, especially those related to possible fracture in the bone, such as fracture strength and fracture energy, etc. [458]. Further studies would be required to develop a more genuine remodelling algorithm in the mandibular reconstruction once specific clinical data is available

Third, it is known that crack nucleation is an important process in fatigue failure which exhibits different crack growth rates with the further propagation stage; and the initial crack length was used to separate these two stages [459]. Owing to the inherent computational limitations, one simplification in this study is that the initial crack length is fairly small which could be classified as short fatigue crack growth problem. Some literature studies indicated that short cracks normally exhibited a higher crack growth rate compared to long cracks with the same level of stress intensity applied [417, 418]. Further efforts are needed to more precisely identify the initial crack length in the reconstruction process, thereby gaining a better understanding of the detailed crack nucleation process.

Consequently, it is recommended that further study should focus on a more realistic prediction of fatigue life in fixation plates through correlation with clinical follow-up subject

to an ongoing measurement of physiological loads and incorporating a more genuine remodeling algorithm.

7.5 Conclusion

This study proposed an XFEM based method to mimic fatigue crack propagation in the fixation plate for a fibula free flap (FFF) based mandibular reconstruction by considering the ongoing bone remodeling effect. It was found that a high biting force can lead to fatigue failure of plate and further, cause significant bone resorption around the crack site. The posterior thinner region around the plate holes has been identified as the most vulnerable area to initiate the cracks. However, when the biting force did not exceed a physiological limit, the simulation suggested that positive remodelling of grafted bone would gradually take more mechanical loading and be of a significant bearing on the fatigue life of fixation plates, substantially extending the lifespan of the plates, in turn stabilizing the reconstruction system. A strong ongoing interaction between fatigue cracking and bone remodelling was established in this study. Such a significant coupling effect thus allows us to draw some clinical guidelines for design optimization of the patient-specific prosthetic system to better ensure the longevity.

Chapter 8: Concluding remarks and future perspective

8.1 Concluding remarks

This thesis investigated biomechanical fracture behaviours in both mineralized and prosthetic materials based on the XFEM framework. The key outcomes achieved within this study are summarized in the following:

Mineralized tissues, such as teeth and bone, play an important role in sustaining the physiological load owing to their high harness and stiffness. However, due to their high hydroxyapatite composition, teeth and bones are relatively brittle biomaterials that have a high susceptibility to mechanical failure. Chapter 3 and Chapter 4 were focused on fracture responses in the human enamel under simulated occlusal loadings. Chapter 3 investigated the effect of anatomical variables, such as fissure morphology, cuspal angle and the enamel material properties of enamel, on the fracture resistance. Overall, the outcomes of this study explain how the interplay of compositional and structural features of enamel in the fissural area contribute to the resistance of the human tooth against masticatory forces. According to the clinical studies, caries and wear are two tooth level conditions which have been commonly observed in cracked tooth. Caries is a plaque induced phenomenon which involves the dissolution of crystal structure of hydroxyapatite in enamel and dentine. Demineralized enamel displays higher porosity, decreased mineral concentration and diminished material properties. Chapter 4 explored the effect of occlusal wear and different types and degrees of caries on the mechanical performance and structural integrity of posterior teeth. The finding

of this chapter demonstrated that the presence of fissural caries, if not treated (either with remineralization, resin infiltration or restoration), can be a major risk factor in the initiation of tooth fracture. The application of a conservative treatment with resin infiltration can be an effective approach in prevention of further mechanical failure of demineralized enamel.

To replace the diseased or injured mineralized tissues, prosthetic materials are largely focused in the areas of dental and osteo clinical applications. Dental restorative materials have been extensively employed in prosthetic dentistry. Ceramic materials present numerous favourable characteristics including biocompatibility and excellent potential to simulate the optical characteristics of natural teeth. Chapter 5 performed an *in-silico* fracture analysis to investigate the fracture behaviours of ceramic dental crowns in relation to the design parameters and material properties. In-vitro fracture tests and fractographic analysis of dedicated models were also performed to validate the findings of the XFEM simulation. Comparing the critical load of crack initiation for different models with the maximum biting force revealed that for the studied monolithic materials, an optimum combination of design parameters in terms of tooth conservation and fracture resistance is determined. Among various CAD/CAM materials, zirconia crowns exhibited sufficient strength for a more conservative design with less thickness. Based on the simulation results, a mathematical formula was proposed to express the relationship between the fracture load and the geometrical factors of crowns, which could provide significant indicators for clinicians and technicians in designing dental crowns.

In addition to the dental industry, applications of osteofixation/osteosynthesis devices, such as fixation plates, are considered fundamental to stabilize various treatments of bone defect for promoting osteointegration and reconstruction. However, clinical observations and

specialized literature have revealed that prosthetic fixation devices are often subject to high stress, leading to fracture by cyclic fatigue failure. In Chapter 5, a XFEM based computational approach is proposed to study the fatigue crack propagation and lifespan in the fixation plates. The numerical analysis is validated by comparing with the experimental and/or clinical results. The results divulge the importance of the tissue ingrowth and bone healing to the fatigue life of fixation plates. The findings from this work would be used as a clinical guideline and beneficial to design and optimize reconstruction devices to ensure durability. According to the computational framework developed in Chapter 5, the ongoing bone remodelling algorithm was added to the XFEM based procedure, which made it possible to investigate the interaction between bone's remodelling and fatigue damage of prosthetic reconstruction plate. The changing mineral density and Young's modulus of bone were predicted in a step-wise fashion based upon Wolff's law, which is correlated with specific clinical follow-up. The effects of masticatory forces measured over time on the fatigue life of fixation plate and bone remodelling were also analyzed. The simulation results indicate that appropriate remodelling of grafted bone could extend the fatigue life of fixation plates in a positive way. However, the healing associated rising occlusal load could lead to fixation plate fatigue fracture and potentially cause severe bone resorption. It is anticipated this approach will provide new insight for design of prosthetic devices and guide the optimal design of patient-specific prosthesis to ensure their longevity.

8.2 Future work

This thesis demonstrated the XFEM as a powerful tool to analyse the fracture behaviours of the brittle biomaterials, and successfully tackled some structural longevity matters in the various biomedical applications. However, there are still some limitations and challenges remain to be addressed, as follows:

One notable limitation of this thesis is the exclusive focus on fracture modelling, which tends to emphasize brittle failure mechanism. The thesis does not delve into the plastic deformation and viscous behaviour exhibited by mineralized and prosthetic biomaterials under certain loading conditions. Considering the permanent and/or time-dependent deformation is essential for understanding the response to the dynamic and repeated loading. Another limitation is that the current thesis does not consider the fracture initiation and propagation in a microscopic level. A prospective avenue for future research could involve delving into the microscopic mechanisms governing the failure of mineralized tissue and synthetic biomaterials. With the help of the high-resolution microscopic techniques, such as Micro-CT, SEM, TEM, etc., it is able to accurately capture the micro/nano structures of the bone and teeth. Based upon the images from such techniques, a more accurate imaged-based FE model can be created and has great potential to precisely simulate the cracking process at the relatively small length scale.

Comprehensive understanding about the role of hierarchical structure of the mineralized tissue on fracture is a major research area in biomedical engineering field. Combining the fine scale models (nano or micro-scale) and macroscopic behaviour are essential to mimic the more realistic fracture process. Hence, one future direction of research is the establishment of

fracture models in multiscale methods. The main challenges of multiscale methods in the future will be the development of techniques to transfer length scales when damage occurs, choosing the suitable discretization. Another challenge that still remain is to overcome the high computational cost, especially in the application of computational design.

Additive manufacturing techniques (3D printing) offers exceptional advantages on fabricating highly sophisticated architectures in prosthetic industry. However, the printing quality still remains some concerns especially for the bioactive ceramics, such as HA. Some experimental study suggested that the printed ceramics exhibited an anisotropic mechanical property due to the layer-by-layer forming mode. In addition, some flaws/cracks can be observed which caused by the thermal stress during sintering process. A high-fidelity FE model could be used to simulate thermal loading and get a more inclusive understanding of the anisotropic behaviour and crack formation induced by the thermal loadings during the fabrication and post-processing process.

Probabilistic failure prediction of brittle biomaterials, considering its inherent stochastic properties, is of critical importance for computational biomedical engineering. The dual high-dimensionality model for both physics modelling and uncertainty quantification is required to accurately represent the voxel-level behaviour, such as fracture initiation. Machine learning techniques, such as artificial neural networks (ANN), have been effectively used for complex problems in engineering and material science. The approach that combines physics-based models and neural networks shows the potential to serve as a surrogate model for probabilistic analysis. The physics-based model could provide a foundation for understanding the underlying principles of fracture behaviour. Then, neural network techniques are employed to represent complex relationships within the physics-based model, thereby

predicting crack initiation and propagation. This approach shows promising applications in predicting fracture behaviours in mineralized and prosthetic materials owing to its excellent reliability, accuracy, and robustness.

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